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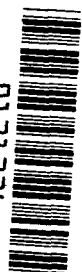


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NUMERICAL PROCEDURES FOR CALCULATING REAL FLUID PROPERTIES OF NORMAL AND PARAHYDROGEN

by Fredric N. Goldberg and Angela M. Haferd

Lewis Research Center

Cleveland, Ohio



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NUMERICAL PROCEDURES FOR CALCULATING REAL FLUID PROPERTIES OF NORMAL AND PARAHYDROGEN

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Lewis Research Center

SUMMARY

Numerical procedures are described for calculating real fluid properties of normal or parahydrogen. The library of single function calls can be used efficiently without initial estimates. When physical conditions are known, engineering estimates of density may be included for additional speed in calculation.

Each of the procedures is designed to calculate a specified function of one or two input parameters. Independent variables consist of the combinations temperature-density, pressure-density, temperature-pressure, enthalpy-pressure, or entropy-pressure. Ideal and saturation properties may also be calculated as functions of either temperature or pressure.

The program is written in separate modules that can be modified easily in the future to include new data. These modules can be used as a subset of functions when computer space is not available for the entire library in complex programs.

The discussion includes techniques used, resolution of inherent physical and mathematical problems, and consistency of results based on National Bureau of Standards data. Computer time and storage estimates are given with a manual of instructions for the programmer. A listing of the program is included as used in the library of functions at the Lewis Research Center.

INTRODUCTION

Present research effort in advanced propulsion systems involves the use of molecular hydrogen as both a propellant and a coolant. The performance analysis of such systems as regeneratively cooled rocket engines requires accurate knowledge of transport and thermodynamic properties in both the liquid and the vapor phase.

Several methods have been published (refs. 1 to 4) for specific applications such as

theoretical analysis (ref. 3) or table computation (ref. 4). In the procedures used in reference 3, close initial estimates are important for convergence. These predictions can be difficult for a user to furnish, and an incorrect estimate can cause the calculation to go out of bounds or iterate indefinitely. In tabular methods (ref. 4), inconsistencies result from interpolations across phase boundaries. Multiple function calls used in reference 4 for increased speed are not in a form suitable for writing complex engineering expressions where single functions are designated as parameters.

In reference 2 the correlations proposed for recent National Bureau of Standards (NBS) tables are extremely difficult to program and require more computer storage than is available when library systems are used. The equation of state proposed in reference 1 by NBS provides a high degree of consistency except in the critical region and for temperatures above 400° K. With modifications and additions in these areas, this equation of state can be used effectively. Related correlations from references 1, 2, 5, and 6 were incorporated in the procedures described in the present report.

The library of functions presented by the authors is currently in general use at the Lewis Research Center for normal or parahydrogen, as required in actual use. The temperature ranges from 14° to 1500° K, and the pressure ranges from 0.1 to 340 atmospheres (approximately 0.1×10^5 to 340×10^5 N/m²). Typical results for all functions except specific heat give a consistency of the order of 0.02 to 0.05 percent in comparison with tabulated NBS data.

The method used herein follows systems programming practice to simplify effort for the user. A single function is specified, and no initial estimate is required. Phase boundaries are automatically defined in all the procedures. The library is in the form of separate modules that can be updated as new data are obtained.

This report presents all pertinent material used in developing the programs of the library. Instructions for use of the functions are given in appendix A. Although the user merely needs to specify the functions as listed in actual application, the report is written to provide the scientific programmer with equations and derivations for reference purposes. For those interested in programming techniques and the solution of the physical problems, these details of the system are developed. The FORTRAN IV program listing in appendix B gives further details for a closer examination and provides coefficients and constants that are not in the text.

SYMBOLS

A, B, C, D, F	constants
C_O	sonic velocity
C_p	specific heat at constant pressure

C_{sl}	specific heat of saturated liquid
C_v	specific heat at constant volume
H	enthalpy
K	thermal conductivity coefficient
m	molecular weight
P	pressure
P_{crit}	critical pressure, 12.77 atm; 1.29392×10^6 N/m ²
R	gas constant
S	entropy
T	temperature
T_{crit}	critical temperature, 32.984 ^o K
V	volume
Z	compressibility factor, $P/\rho RT$
γ	specific heat ratio, C_p/C_v
μ	shear coefficient viscosity
ρ	density
ρ_{crit}	critical density, 0.0152672 (g)(mole)/cm ³ ; 30.7744 kg/m ³
σ	defined by eq. (3)

Subscripts:

crit	critical value
cs	program constant
h	high
id	ideal gas
l	low
lim	limit
liq	liquid
o	base line reference
sat	saturated line
sl	saturated liquid

sv saturated vapor
x mixture under vapor dome

PRESSURE-TEMPERATURE-DENSITY PROCEDURES

Basic Equations

Equations of state are used to represent the basic physical relation among density, pressure, and temperature.

A modified Benedict-Webb-Rubin equation of state (ref. 1) is used for temperatures up to and including 400° K:

$$P = a_1 \rho T + \rho^2 \left(a_1 a_2 T + a_3 + \frac{a_4}{T} + \frac{a_5}{T^2} + \frac{a_6}{T^4} \right) + \rho^3 \left[a_7 a_1 T + a_8 + \left(\frac{a_{10}}{T^2} + \frac{a_{11}}{T^3} + \frac{a_{12}}{T^4} \right) e^{-a_{17} \rho^2} \right] \\ + a_9 T \rho^4 + \rho^5 \left(\frac{a_{13}}{T^2} + \frac{a_{14}}{T^3} + \frac{a_{15}}{T^4} \right) e^{-a_{17} \rho^2} + a_{16} \rho^6 \quad (1)$$

The coefficients a_1 to a_{17} are specified in two groups for regions designated as either vapor or liquid. Combinations of temperature and density identify the two regions.

For temperatures above 400° K, a high-temperature equation of state from reference 5 is used:

$$P = RT\rho \exp \left[B(T)\rho + C(T)\rho^2 \right] \quad (2)$$

where

$$B(T) = B_1 T^{-1/4} + B_2 T^{-3/4} + B_3 T^{-5/4}$$

and

$$C(T) = C_1 T^{-3/2} + C_2 T^{-2}$$

Equations derived from reference 1 are used to evaluate the two-phase region.

Equations (3) and (4) define the liquid boundary:

$$P_{\text{sat}} = P_{\text{crit}} - [\sigma(T)]^3 \sum_{n=0}^4 b_n [\sigma(T)]^n \quad (3)$$

$$\sigma(T) = \sum_{n=1}^4 a_n (T_{\text{crit}} - T)^{n/3}$$

$$\rho_{\text{sl}} = \rho_{\text{crit}} + \sigma(T) \quad (4)$$

The saturated vapor boundary is defined as the values of density at the intersection of isotherms (eq. (1)) with saturation pressure (eq. (3)). An ideal gas is defined as one that is described by the perfect gas law, where $P = R\rho T$, but has a temperature-dependent specific heat.

Region Determination and Initialization

All property evaluations involving equations of state must be preceded by a region-finding process to determine which equation of state applies. The region-finding process also provides additional information required to initialize iterations and to specify boundary values. These regions are described in the diagrams of figure 1.

Since all state equations used give pressure as a function of temperature and density, the combination of temperature and density as independent variables directly determines the region. For the cases where independent variables are pressure and density, or pressure and temperature, indirect methods of region determination have to be made. These implicit determinations depend on the property that both derivatives $(\partial P / \partial T)_{\rho}$ and $(\partial P / \partial \rho)_T$ are nonnegative.

Calculation Procedure

The procedures for evaluating the pressure-density-temperature surface are programmed in the form

$$P(\rho, T) \quad \text{pressure}$$

$T(P, \rho)$ temperature

$\rho(T, P)$ density

The evaluation of pressure is a direct substitution of the values of density and temperature in the appropriate state equation.

Temperature and density procedures involve a method of successive approximations in which a sequence of trial values is generated by a Newton type iteration:

$$T_{n+1} = T_n - \frac{P(T_n, \rho) - P}{\frac{\partial P}{\partial T}(T_n, \rho)}$$

$$\rho_{n+1} = \rho_n - \frac{P(T, \rho_n) - P}{\frac{\partial P}{\partial \rho}(T, \rho_n)}$$

Indicated partial derivatives are formal evaluations of derivatives of the state equation applicable for the region.

The values of iterants are governed by algorithms that recognize the behavior of the particular function and its derivatives in each region of interest. This technique prevents values from exceeding the range indicated by the region finding process and guarantees convergence.

Critical Region Calculations

In the vicinity of the critical region, the density calculation is extremely unstable. Large errors occurred in calculating functions and derivatives of the equation of state. To eliminate this problem, an empirical correlation was substituted. Two sets of density values ρ_l and ρ_h were fit empirically for isotherms in the temperature range between 32.5° and 35° K. The variation of density with pressure in this region was then described by an interpolation formula. The criteria used to isolate the region are symbolically shown in figure 2.

The resulting representation used for the density procedure is summarized as follows:

For $32.5 < T < T_{\text{crit}}$:

$$P(\rho_l, T) < P < P_{\text{sat}}(T)$$

$$\rho = \frac{(\rho_{\text{sv}} - \rho_l)(P - P_{\text{sat}})}{[P_{\text{sat}} - P(\rho_l, T)]} + \rho_{\text{sv}}$$

$$P_{\text{sat}}(T) < P \leq P(\rho_h, T)$$

$$\rho = \frac{(\rho_h - \rho_{\text{sl}})[P - P(\rho_h, T)]}{[P(\rho_h, T) - P_{\text{sat}}]} + \rho_h$$

For $T_{\text{crit}} \leq T < 35^\circ \text{ K}$:

$$P(\rho_l, T) < P < P(\rho_h, T)$$

$$\rho = \frac{(\rho_h - \rho_l)[P - P(\rho_h, T)]}{[P(\rho_h, T) - P(\rho_l, T)]} + \rho_h$$

State equation (1) is used to calculate the values $P(\rho_l, T)$ and $P(\rho_h, T)$ with the use of liquid or vapor coefficients as indicated. The result of this technique is a distortion of the vapor-liquid dome to avoid numerical difficulties and errors.

THERMODYNAMIC AND TRANSPORT PROCEDURES

Functions of Temperature and Pressure

The first group of four procedures for thermodynamic and transport properties is programmed in the form generally used in data reduction. Pressure and temperature are the given parameters:

$H(P, T)$	enthalpy
$S(P, T)$	entropy
$C_p(P, T)$	specific heat, also includes C_v and C_o
$\mu(P, T)$	viscosity, also includes thermal conductivity K

In each of these procedures, density $\rho(P, T)$ is first calculated, which automatically identifies the region. Then the property is calculated by combining a function of temperature only with an isothermal deviation term. (See appendix C for details.) The deviation term reflects the real gas effects, and it is represented by either functions of the appropriate state equation or other empirical correlations. These relations are summarized as follows:

$$H = H(T, \rho_0) + \left[\frac{P(T, \rho)}{\rho} - \frac{P(T, \rho_0)}{\rho_0} \right] + \int_{\rho_0}^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho$$

$$S = S(T, \rho_0) - \int_{\rho_0}^{\rho} \left[\frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho$$

$$C_v = C_v(T, \rho_0) - T \int_{\rho_0}^{\rho} \left[\frac{1}{\rho^2} \left(\frac{\partial^2 P}{\partial T^2} \right)_{\rho} \right]_{\rho} d\rho$$

$$C_p = C_v + \frac{T \left(\frac{\partial P}{\partial T} \right)^2}{\rho^2 \left(\frac{\partial P}{\partial \rho} \right)_{\rho}}_{\rho}$$

$$C_o = \left[\frac{C_p \left(\frac{\partial P}{\partial \rho} \right)_{\rho}}{C_v} \right]^{1/2}$$

$$\mu = \mu_o(T) + \mu_1(T, \rho)$$

$$K = K_o(T) + K_1(\rho)$$

All derivatives and integrals in these equations are evaluated in closed form from the equations of state.

Functions of Pressure and Enthalpy or Entropy

Two procedures for calculating temperature and density for a given value of pressure with enthalpy or entropy are of the form $T(P, H)$ and $T(P, S)$.

Since the equations of state are represented as explicit functions of ρ, T , it is possible to express H or S as a function of the same two parameters. These calculations involve simultaneous solution of two nonlinear equations. To guarantee a convergent sequence, the problem was linearized. A sequence of temperatures is generated with the use of a one-dimensional Newton type iterative scheme. An intermediate calculation of density is performed for each temperature and pressure. Initial values of temperature are chosen through an algorithm that avoids crossing region boundaries. Infinite loops in the computation are thus avoided for the intermediate iterates.

The initial region calculation in this case may determine that the state point (H, P) or (S, P) lies within the two-phase region. When this occurs, the problem is reduced to calculating the saturation temperature corresponding to the given pressure. The density for the mixture region is then calculated from the following equations that represent an average density variation with mixture quality:

$$\rho_x = \frac{\rho_{sv}\rho_{sl}}{[x\rho_{sl} + (1 - x)\rho_{sv}]}$$

where

$$x = \frac{H - H_{sl}}{H_{sv} - H_{sl}}$$

or

$$x = \frac{S - S_{sl}}{S_{sv} - S_{sl}}$$

Functions of One Parameter

To facilitate the programming of data reduction problems in which only one parameter can be measured and a given phase value of the fluid is to be assumed (such as saturated liquid, saturated vapor, mixture quality, etc.), procedures are included to calculate saturated or ideal values of the following properties as functions of temperature: $P_{\text{sat}}(T)$ is given by equation (3), $\rho_{sl}(T)$ by equation (4), $\rho_{sv}(T)$ occurs at the intersection of equations (1) and (3),

$$C_{p, id}(T) = A_{id} + B_{id}T + C_{id}T^2 + D_{id}T^3 + E_{id}T^4 + F_{id}T^5$$

$$H_{id}(T) = H_{id}(T_o) + \int_{T_o}^T C_{p, id}(T) dT$$

$$S_{id}(T) = S_{id}(T_o) + \int_{T_o}^T \frac{C_{p, id}(T)}{T} dT$$

where $S_{id}(T_o)$ is evaluated at a pressure of 1 atmosphere (1.01×10^5 N/m²)

$$H_{sv}(T) = H_{id}(T) + \frac{P_{sat}}{\rho_{sv} - RT} + \int_0^{\rho_{sv}} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

$$S_{sv}(T) = S_{id}(T) - R \ln(RT\rho_{sv}) + \int_0^{\rho_{sv}} \left[\frac{R}{\rho} - \frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

$$H_{sl}(T) = H_{sl}(T_o) + \int_{T_o}^T C_{sl}(T) dT + \int_{\rho_{sl}(T_o)}^{\rho} \frac{dP}{\rho} \quad (5a)$$

where

$$C_{sl}(T) = \frac{A_{cs}T}{(T_{crit} - T)^{1/2}} + B_{cs} + C_{cs}T + D_{cs}T^2 + E_{cs}T^3 \quad (5b)$$

$$S_{sl}(T) = S_{sl}(T_o) + \int_{T_o}^T \left[\frac{C_{sl}(T)}{T} \right] dT$$

$$C_{v_{sv}}(T) = C_{p, id}(T) - R + \int_0^{\rho_{sv}} \left(\frac{\partial C_v}{\partial \rho} \right)_T d\rho$$

$$C_{v_{sl}}(T) = C_v(\rho_1, T) + \int_{\rho_1}^{\rho_{sl}} \left(\frac{\partial C_v}{\partial \rho} \right)_T d\rho$$

where $C_v(\rho_1, T)$ is heat capacity at constant density, as tabulated in reference 2, and $\rho_1 = 0.037821$ gram-mole per cubic centimeter (or 76.237 kg/m^3). The quantities $C_{p_{sl}}$ or $C_{p_{sv}}$ and C_o are calculated with the use of relations summarized for functions of temperature and pressure. However, caution must be exercised in the use of C_p and C_o at the saturation line, because the values returned are calculated as limits as the density approaches saturation but do not reflect the physical fact that the actual value of the property may become unbounded at the onset of cavitation or two-phase flow.

In addition to the given functions of temperature, a procedure is included for calculation of saturation temperature based on an input pressure.

The quantity $T_{sat}(P)$ is obtained by an iterative calculation based on an empirical equation from reference 3:

$$P_{sat} = \exp F(T_{sat}) \quad (6)$$

where

$$F(T_{sat}) = A_{ts} + \frac{B_{ts}}{T_{sat} + C_{ts}} + D_{ts} T_{sat}$$

EFFECT OF COMPOSITION ON PROPERTIES OF NORMAL OR PARAHYDROGEN

The primary use of the library of property functions is for parahydrogen composition. An option is included for normal hydrogen composition in the vapor region in the procedures for enthalpy, entropy, specific heat, and transport properties. When the composition is 75-percent orthohydrogen and 25-percent parahydrogen, the gas is considered to be in the normal mode. In the liquid region, the presence of normal composition would be extremely rare in actual application and is not considered.

The pressure-density-temperature surface for hydrogen is nearly independent of orthopara percentage. State equations, real gas deviation, and excess function can be treated as independent of the effect of composition. However, the major difference in property values is in the base line or ideal gas value. In the procedures for enthalpy, entropy, and specific heat, provision is made to calculate the base effects for either nor-

mal or paracomposition as designated by the user.

The effect of composition on transport properties is significant only in thermal conductivity. The proper value of the ideal gas specific heat is used to reflect the difference in composition between normal and para. In the viscosity function, the effect is not significant but the programming of the two functions is related in the procedure call, and the option is used for normal or para.

Liquid hydrogen is considered to be equivalent to para in the research applications in heat transfer for which the functions are used. However, a relatively good estimate of liquid-hydrogen normal functions can be derived by correcting values for parahydrogen by the difference in ideal gas values. The library of functions includes ideal gas properties for this purpose and for other uses.

USE OF PROCEDURES AND RESULTS

Consistency and Validity of Results

Error analysis is considered in two categories. The first is internal consistency within the group of functions, and the second is comparison of results with reference values or source data. Physical and mathematical consistency is considered most important in the experimental and analytical computations. Misleading physical results must be prevented, such as an isobaric increase of enthalpy indicating a temperature drop or density rise. The mathematical consistency among the related functions and their inverses is kept to within approximately 0.1 percent. Slightly larger errors occur near the critical pressure-temperature point that must be recognized in any application. Certain tolerances are also used at the saturated liquid boundaries for mathematical reasons.

Comparison of results obtained for pressure-density-temperature relations with references 2, 5, 7, and 8 shows agreement to within approximately 0.02 percent for all regions except critical. The error of approximation compares with the experimental accuracy represented in the available sources of data. In some functions, such as enthalpy and entropy, the agreement within the published sources varies slightly because of reference conditions. The specific-heat function is uncertain in the saturated region, and near the critical point it becomes unbounded. This function changes rapidly at other low pressures, as shown in figure 3. However, overall results compare well at all points, except the critical region, with errors within 0.5 to 2.0 percent.

The agreement for transport properties is completely consistent with recent information (refs. 3, 6, 9, and 10) and the same mathematical method is used with identical empirical relations. However, the validity of referenced correlations for viscosity and

thermal conductivity is not definitely established at present. Computer-generated plots of the properties of parahydrogen as represented in this report are included in figures 3 to 8.

Execution Time for Function Calls

For programming applications, the average time estimate for each function call involving state equations and iteration is at the rate of approximately 200 per second. Calculation speed can be increased by a factor of 3 to 4 when close estimates of density are furnished in any function of temperature and pressure. Successive calculations of functions in which there are only small variations in density also automatically provide increased speed. When density is calculated along with another function, it is also provided as a secondary result in common. Other related functions are also grouped that can be computed simultaneously, such as viscosity-conductivity, or a combination of specific heats C_p and C_v , and sonic velocity C_o .

Explicit functions, such as pressure in state equations, or saturated region relations and ideal functions, are calculated at a rate of several thousand per second.

Programming Use of Library of Functions

The list of function calls with instructions for programming is given in appendix A. The prefix identifying the library represents the system of units being used. The letters BW refer to the internal library units corresponding to the Benedict-Webb-Rubin equation of state (eq. (1)), which is in the calorie-gram-centimeter system. The particular function is specified by a number according to the listed parameters given.

For input and output in British thermal units, the prefix BT is used in the function call. The prefix BI is used for input-output in the SI system. The function number is also modified to indicate that the composition of the hydrogen is normal rather than parahydrogen.

CONCLUDING REMARKS

The procedures presented have been applied at the Lewis Research Center effectively in various experimental and theoretical research projects. The applications included large programs, such as convective cooling analysis, reduction of data from nuclear engine simulations, rocket engine design and performance calculations, and correlations for

experiments with pressurized tank storage and pumping of hydrogen.

Evaluations of performance parameters have been made efficiently and smoothly proving the consistency and versatility of the functions used. In comparison with National Bureau of Standards tables, the properties calculated were more consistent than those obtained with the use of other methods. Improvements were made especially in the critical region and in the liquid-vapor phase boundary definition.

The techniques originated by the authors provide solutions for similar problems that would be encountered in applying state equations for properties of other fluids.

Lewis Research Center,

National Aeronautics and Space Administration,

Cleveland, Ohio, September 13, 1967,

125-23-02-10-22.

APPENDIX A

PROGRAMMING INSTRUCTIONS FOR HYDROGEN PROPERTIES

Calling Sequence

The programming function call is written in the form of either BW(N, P1, P2), BT(N, P1, P2), or BI(N, P1, P2). The prefix designates which system of units is to be used in the conversion: BW is used for cgs units (calorie-gram-centimeter-second) system, BT is used for British thermal units system, and BI is used for the SI system.

The integer N specifies which thermodynamic property is to be computed. Parameters P1 and P2 are input combinations depending on N, as shown in table I.

Related output is also given in NAMED COMMON from certain procedures.

TABLE I. - VALUES OF N^a FOR SELECTION OF THERMODYNAMIC PROPERTY

[For British thermal units, use prefix BT in place of BW; for SI units, use prefix BI.]

Function call	Designated function	Related output				
		BWX	BWD	BWCVGL	BWCOND	BWCO
BW(1, T, P)	Density, D	X	D	---	----	---
BW(2, T, P)	Enthalpy, H	X	D	---	----	---
BW(3, T, P)	Entropy, S	X	D	---	----	---
BW(4, H, P)	Temperature, T	X	D	---	----	---
BW(5, S, P)	Temperature, T	X	D	---	----	---
BW(6, T, P)	Specific heat, CP	X	D	CV	----	CO
BW(7, T, P)	Viscosity, μ , $\times 10^4$	X	D	---	$K \times 10^4$	---
BW(8, T, D)	Pressure, P	X	---	---	----	---
BW(9, D, P)	Temperature, T	X	---	---	----	---
BW(10, T, O)	Saturation pressure, P	---	---	---	----	---
BW(11, P, O)	Saturation temperature, T	---	---	---	----	---
BW(12, T, O)	Density of saturated liquid	---	---	---	----	---
BW(13, T, O)	Density of saturated vapor	---	---	---	----	---
BW(14, T, O)	Specific heat of ideal gas	---	---	---	----	---
BW(15, T, O)	Specific heat of saturated liquid	---	D	CV	----	CO
BW(16, T, O)	Specific heat of saturated vapor	---	D	CV	----	CO
BW(17, T, O)	Enthalpy of ideal gas	---	---	---	----	---
BW(18, T, O)	Enthalpy of saturated liquid	---	---	---	----	---
BW(19, T, O)	Enthalpy of saturated vapor	---	D	---	----	---
BW(20, T, O)	Entropy of ideal gas	---	---	---	----	---
BW(21, T, O)	Entropy of saturated liquid	---	D	---	----	---
BW(22, T, O)	Entropy of saturated vapor	---	D	---	----	---

^aFor normal hydrogen, N is replaced by N + 200.

Physical Units

In table II the physical units and symbols used in the various function calculations are presented.

TABLE II. - SYSTEM OF UNITS FOR VARIOUS PROPERTIES

Property	Symbol	Physical units		
		BW	BT	BI
Temperature	T	$^{\circ}\text{K}$	$^{\circ}\text{R}$	$^{\circ}\text{K}$
Pressure	P	atm	lb/sq in.	N/m^2
Density	D	g/cc	lb/cu ft	kg/cu m
Enthalpy	H	cal/g	Btu/lb	J/kg
Entropy	S	$\text{cal}/(\text{g})(^{\circ}\text{K})$	$\text{Btu}/(\text{lb})(^{\circ}\text{R})$	$\text{J}/(\text{kg})(^{\circ}\text{K})$
Specific heat at constant pressure	C_p	$\text{cal}/(\text{g})(^{\circ}\text{K})$	$\text{Btu}/(\text{lb})(^{\circ}\text{R})$	$\text{J}/(\text{kg})(^{\circ}\text{K})$
Specific heat at constant volume	C_v	$\text{cal}/(\text{g})(^{\circ}\text{K})$	$\text{Btu}/(\text{lb})(^{\circ}\text{R})$	$\text{J}/(\text{kg})(^{\circ}\text{K})$
Sonic velocity	C_O	cm/sec	ft/sec	m/sec
Viscosity	μ	$\text{g}/(\text{cm})(\text{sec})$ or $\text{P} \times 10^4$	$[\text{lb}/(\text{ft})(\text{sec})] \times 10^4$	$[(\text{N})(\text{sec})/\text{sq m}] \times 10^4$
Thermal conductivity	K	$[\text{cal}/(\text{cm})(\text{sec})(^{\circ}\text{K})] \times 10^4$	$[\text{Btu}/(\text{ft})(\text{sec})(^{\circ}\text{R})] \times 10^4$	$[\text{J}/(\text{m})(\text{sec})(^{\circ}\text{K})] \times 10^4$
Number designating region	X	Liquid (-1), vapor (2), or liquid-vapor mixture (0-1)	-----	-----

In the liquid-vapor two-phase region, x is equal to the quality of the fluid.

Applicable Range of Validity

The range for which the function calls are valid can be summarized in terms of temperature and pressure approximately as follows:

Temperature:

$^{\circ}\text{K}$	14 to 1500
$^{\circ}\text{R}$	25 to 2700

Pressure:

atm	0.1 to 340
psi	1 to 5000
N/m^2	10 000 to 340×10^5

Intermediate Results in NAMED COMMON

Depending on the choice of N, the following properties result in common:

BTX, BWX, or BIX	quality or region
BTD, BWD, or BID	density
BTCVGL, BWCVGL, BICVGL	specific heat at constant volume
BTCOND, BWCOND, BICOND	thermal conductivity
BTCO, BWCO, or BICO	sonic velocity

NAMED COMMON is required in the main program whenever any of this related output is to be used, and is declared in double precision as follows:

COMMON/BWDXCK/BWD, BWX, BWCVGL, BWCOND

COMMON/BTDXCK/BTD, BTX, BTCVGL, BTCOND, BTCO

COMMON/BWSONV/BWCO

COMMON/BIDXCK/BID, BIX, BICVGL, BICOND, BICO

DOUBLE PRECISION BTD, BTX, BTCVGL, BTCOND, BTCO

DOUBLE PRECISION BWD, BWX, BWCVGL, BWCOND, BWCO

DOUBLE PRECISION BID, BIX, BICVGL, BICOND, BICO

Normal Hydrogen

For properties of normal hydrogen, the value of N given in table I is replaced by $N + 200$ in all cases where the region is applicable as vapor. If the programmer specifies normal hydrogen in the function call, the value returned when the region is not found to be vapor will be for parahydrogen composition.

Saturation Conditions

If saturation conditions are determined to exist where pressure and temperature are

the independent variables, the results returned are those corresponding to saturated liquid conditions.

Special Properties

In any function that uses temperature and pressure as independent variables, an engineering estimate of density may be provided. This value is put in BWD, BTD, or BID depending on the system of units used.

In general, a single result is returned as the value of an expression. For example, in computing the free energy $H - TS$ given P and T , the programmer writes

$$F = BW(2, T, P) - T \times BW(3, T, P)$$

In this case, the intermediate results $H = BW(2, T, P)$ and $S = BW(3, T, P)$ are not automatically stored.

Computer Storage Requirements

Approximately 9000 (decimal) computer stores are required.

APPENDIX B

PROGRAM LISTINGS

Grouping of Related Modules

Group (1) BW program used for cgs function calls

Group (2) Basic P , ρ , T group (requires module of group 1):

BWDENS, BWBLOK, LIQUID, VAPOR,

PK, PPK, COEF, BWPSAT, BWROSV,

ROKSL, BWTSAT, DPDT, BWTEMP, BWPRES

Group (3) Thermodynamic group of H , S , C_p functions (requires modules of groups 1 and 2):

PARALO, PARAHI, NORMLO, NORMHI, COEFID,

BWCPIG, BWHIDG, BWSIDG, BWSSTL, BWHSTL,

BWSSV, SKSL, BWSSL, HKSV, HKSL, SKSV,

HDEV, BWHSV, BWHSL, SDEV, BWENHY,

BWERPY, BWTOFH, BWTOFS, BWFD2, BWCPGL

Group (4) Transport properties μ , K for all temperatures and high-temperature functions P , ρ , T , H , S , C_p , C_v , C_o (requires modules of groups 1, 2, and 3):

BWVISC, HTCPIG, HTHIDG, HTSIDG, HTHDEV,

HTENHY, HTSDEV, HTERPY, HTTOFS, HTDPDT,

HTDENS, HTFD2, HTTOFH, HTCPGL, HTTMP, HTPKS

Group (5) BT program used for British thermal units function calls (optional)

Group (6) BI program used for SI units function calls (optional)

Group (7) Function NTAG (optional for omitting tagged data check)

FORTRAN IV Program Listing For Library of Functions

```

$IBFTC BW      DECK
C      SUBPROGRAM USED FOR ALL PROPERTIES IN BW UNITS (CGS) SYSTEM
C      FOR PARAHYDROGEN N=1 ~ 22 OR NORMAL HYDROGEN N=201-222
C      IN CALORIES-GRAM-SECOND SYSTEM. P=.1 - 340 ATM
C      TEMPERATURES 14 TO 1500 DEG KELVIN
      FUNCTION BW(N,P1,P2)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/BWSONV/BWCO
      DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
      DOUBLE PRECISION BWCO
      NUDE = N/100
      T400=400.
      M= N-100*MODE
      BW= P1+P2
      IF (NTAG(BW).NE.0) GO TO 333
      GOTO (1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22),M
333  BWD= BW
      BWX=BW
      IF (M.NE.6) GO TO 334
      BWCVGL=BW
      BWCO=BW
      RETURN
334  IF (M.NE.7) GO TO 335
      BWCOND=BW
335  RETURN
      1 IF(P1.GT.T400) GO TO 101
      BW= BWDENS(P1,P2)
      RETURN
101  BW= HTDENS(P1,P2)
      RETURN
      2 IF(P1.GT.T400) GO TO 102
      BW= BWENHY(P1,P2)
      RETURN
102  BW= HTENHY(P1,P2)
      RETURN
      3 IF(P1.GT.T400) GO TO 103
      BW= BWERPY(P1,P2)
      RETURN
103  BW= HTERPY(P1,P2)
      RETURN
      4 H= BWENHY(400.,P2)
      IF(P1.GT.H) GO TO 104
      BW= BWTCFH(P1,P2)
      RETURN
104  BW= HTTOFH(P1,P2)
      RETURN
      5 S= BWERPY(400.,P2)
      IF(P1.GT.S) GO TO 105
      BW= BWTCFS(P1,P2)
      RETURN
105  BW= HTTOFS(P1,P2)
      RETURN
      6 IF(P1.GT.T400) GO TO 106
      BW= BWCPGL(P1,P2)
      RETURN
106  BW= HTCPGL(P1,P2)
      RETURN
      7 BW= BWVISC(P1,P2)
      RETURN

```

```

      8  IF(P1.GT.T400)GO TO 108
        BW=BWPRES(P1,P2)
        RETURN
108  BW=HTPRES(P1,P2)
        RETURN
      9  P=BWPRES(T400,P1)
        IF(P2.GT.P) GO TO 109
        BW=BWTEMP(P1,P2)
        RETURN
109  BW=HTTEMP(P1,P2)
        RETURN
     10  BW= BWPSAT(P1)
        RETURN
     11  BW= BWTSAT(P1)
        RETURN
     12  BW= ROKSL(P1)*2.0157
        RETURN
     13  BW= BWR0SV(P1)
        RETURN
     14  IF(P1.GT.T400) GO TO 114
        BW= BWCPIG(P1)
        RETURN
114  BW= HTCPIG (P1)
        RETURN
     15  PSAT= BWPSAT(P1)+.001
        BW= BWCPGL(P1,PSAT)
        RETURN
     16  PSAT= BWPSAT(P1)-.001
        BW= BWCPGL(P1,PSAT)
        RETURN
     17  IF(P1.GT.T400) GO TO 117
        BW= BWHIDG(P1)
        RETURN
117  BW= HTHIDG(P1)
        RETURN
     18  BW= BWHSTL(P1)
        RETURN
     19  PSAT= BWPSAT(P1)+.001
        BW= BWHSV(PSAT)
        RETURN
     20  IF(P1.GT.T400) GO TO 120
        BW= BWSIDG(P1)
        RETURN
120  BW= HTSIDG(P1)
        RETURN
     21  BW= BWSSTL(P1)
        RETURN
     22  PSAT= BWPSAT(P1)
        BW= BWSSV(PSAT)
        RETURN
      END
$IRFTC BWDENS  DECK
C      CALCULATES DENSITY IN C.G.S. UNITS AS FUNCTION
C      OF TEMPERATURE AND PRESSURE.  REQUIRES BASIC MODULES BWBLOK,
C      BWPSAT, VAPUR, LIQUID, PK, PPK, COEF, AND ROKSL
      DOUBLE PRECISION FUNCTION BWDENS (T6,P6)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/WORKS/WKS,W1,W2,W3,W4,S

```

```

COMMON/KUNS/TCRIT,PCRIT,ROCRIT,TOL,D41R
DOUBLE PRECISION T6,P6,BWPSAT,ROKSL,PK,PPK
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION WKS,W1,W2,W3,W4,S
DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
LOGICAL ESTD
ESTD= .TRUE.
ROK=BWD/2.0157
ROID=P6/T6/82.082
IF (TCRIT-T6) 2,1,1
1 WKS = BWPSAT (T6)
CALL LIQUID
IF (WKS - P6) 3,3,22
3 IF (P6 - WKS - .0001) 5,4,4
4 XVAL = -1.
BOUNDL=ROCRIT + S
UBOUND=.05
RESTR= .05
IF (T6.GT.32.5) GO TO 44
GOTO 10
5 ROK = ROKSL (T6)
CALL COEF(T6)
WKS= PK(ROK)
XVAL = 0
GOTO 12
2 CALL VAPOR
BOUNDL=0.
UBOUND=.05
XVAL = 2
IF (T6.LT.35.) GOTO 66
IF (P6 - PCRIT) 6,6,7
6 RESTR=ROID
GO TO 10
7 RESTR=.05
10 CALL COEF (T6)
15 DO 11 ITERS=1,10
IF (ESTD) GO TO 1000
16 X = PK(ROK)
WKS=PPK(ROK)
DELTA=(X - P6)/WKS
ROK=ROK - DELTA
IF(DABS(DELTA) - TOL) 12,12,11
11 CONTINUE
GO TO 12
1000 IF (ROK.GT.BOUNDL.AND.ROK.LT.UBOUND)GO TO 16
ROK = RESTR
ESTD= .FALSE.
GO TO 15
60 UBOUND=ROLOW
RESTR=ROID
GO TO 15
22 CALL VAPOR
BOUNDL=ROID
UBOUND=ROCRIT
RESTR=ROID
ROK=ROID
XVAL= 2.
ROLOW= -.043 + .0016* T6
ROHIGH= ROCRIT - S

```

```

    PHIGH= WKS
    CALL COEF(T6)
    PLOW= PK(ROLOW)
    IF(T6.LT.32.5) GO TO 15
    UBOUND=ROLOW
    IF (P6.LT.PLOW) GO TO 6
    GO TO 100
44 ROHIGH= .086 - .002 * T6
    BOUNDL=ROHIGH
    ROLOW= S + ROCRIT
    PLOW = WKS
    CALL COEF (T6)
    PHIGH= PK(ROHIGH)
    IF (P6.GT.PHIGH) GO TO 10
    GO TO 100
66 ROLOW= -.043 + .0016* T6
    ROHIGH= .086 -.002 *T6
    CALL COEF(T6)
    PLOW= PK(ROLOW)
    IF (P6.LT.PLOW) GO TO 60
    CALL LIQUID
    CALL COEF(T6)
    PHIGH= PK(ROHIGH)
    BOUNDL= ROHIGH
    RESTR=.05
    IF (P6.GT.PHIGH) GO TO 15
100 ROK= ROHIGH-(PHIGH-P6)/(PHIGH-PLOW)*(ROHIGH-ROLOW)
    PHIGH= PK(ROK)
12 D= ROK * 2.0157
    BWDENS = D
    BWD = D
    BWX= XVAL
    RETURN
END
$IBFTC BWBLOK DECK
C      PROGRAM CONSTANTS FOR CRITICAL TEMPERATURE, PRESSURE,DENSITY, AND
C      COEFFICIENTS FOR EQUATION OF STATE (1)
    BLOCK DATA
    COMMON/FIXED/MODE,ITERS
    COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
    COMMON/PTD/P,T,D,ROK,DELTA,XVAL
    COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
    COMMON/CVS/CS,CH,FE,U,C,B,AA
    COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
    COMMON/WORKS/WKS,W1,W2,W3,W4,S
    COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
    COMMON/ACOE/A(17)
    COMMON/LCOEF/AL(17)
    COMMON/VCOEF/AV(17)
    DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
    DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
    DOUBLE PRECISION PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
    DOUBLE PRECISION CS,CH,FE,U,C,B,AA
    DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
    DOUBLE PRECISION WKS,W1,W2,W3,W4,S
    DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
    DOUBLE PRECISION A
    DOUBLE PRECISION AL
    DOUBLE PRECISION AV
    DATA (AV(I), I=1,17)/82.08199823,20.62278898,-129279.2029,

```

```

1 -7237230.1370, 115924274.50, -10108798750.,
2 317.62939700, 2581305.9670, 241066.9065, -10703806250.,
3 1016369054000., -19384310020000., 3857308627000.,
4 -675746323600000., 14621146530000000., 52549922590., 1800.100800/
5 , (AL(I), I=1,17)/ 82.08199823, 63.74020840, -353918.0407,
6 -4810952.457, 91278833.49, -8816106422.,
7 -1283.735749, 8076213.444, 1425160.973, 6410245277.,
8 108516291300., -2930340262000., -5235483345000.,
9 -255111438000000., 4732799310000000., 35223277740.0, 1800.100800/
DATA (TCRIT,PCRIT,ROCRIT,TOL)/ 32.98400, 12.7700, .0152672 DO,
1 .00001 DO/
END
$IBFTC LIQUID DECK
SUBROUTINE LIQUID
COMMON/LCOEF/AL(17)
COMMON/ACDEF/A(17)
DOUBLE PRECISION AL,A
DO 77 I=1,17
77 A(I) = AL(I)
RETURN
END
$IBFTC VAPOR DECK
SUBROUTINE VAPOR
COMMON/VCOEF/AV(17)
COMMON/ACDEF/A(17)
DOUBLE PRECISION AV,A
DO 77 I=1,17
77 A(I) = AV(I)
RETURN
END
$IBFTC PK DECK
C PRESSURE FUNCTION OF DENSITY GRAM-MOLE/CC AND COMMON T TERMS
DOUBLE PRECISION FUNCTION PK(RK2)
COMMON/ACDEF/A(17)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION RK2,DEXP
DOUBLE PRECISION A
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
EK= DEXP ( -A(17) * RK2*RK2)
CF= C2 * EK + C1
EF= E1 * EK
PK=(((FF*RK2+EF)*RK2 +DF)*RK2+CF)*RK2 + BF)*RK2+AF)*RK2
RETURN
END
$IBFTC PPK DECK
C PARTIAL DERIVATIVE FOR PRESSURE AND DENSITY
DOUBLE PRECISION FUNCTION PPK(RK3)
COMMON/ACDEF/A(17)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION RK3
DOUBLE PRECISION A
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
PPK= ((((-2.* A(17)*EF*RK3+6.*FF)*RK3+(5.*EF -2.*A(17)*C2*EK))
1 *RK3+4.*DF) *RK3 + 3.*CF) *RK3 + 2.*BF) * RK3 + AF
RETURN
END
$IBFTC COEF DECK
C FUNCTIONS OF TEMPERATURE FOR STATE CALCULATIONS
SUBROUTINE COEF (T1)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK

```

```

COMMON/ACDEF/A(17)
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION A
DOUBLE PRECISION T1
AF = A(1) * T1
BF= AF*A(2) + A(3) + ((A(6)/T1/T1 + A(5))/T1 + A(4))/T1
DF= A(9) * T1
FF= A(16)
C2= ((A(12)/T1 + A(11) )/T1 + A(10) ) / T1/T1
E1= ((A(15)/T1 + A(14))/T1 + A(13) )/T1/T1
C1 = A(7)* AF + A(8)
RETURN
END

$IBFTC BWPSAT DECK
C SATURATION PRESSURE ATM FUNCTION OF TEMPERATURE DEGREES KELVIN
DOUBLE PRECISION FUNCTION BWPSAT (T5)
COMMON/KONS/TCRIT,PCRTT,ROCRIT,TOL,D41R
COMMON/WORKS/WKS,W1,W2,W3,W4,S
DOUBLE PRECISION T5,ROKSL
DOUBLE PRECISION WKS,W1,W2,W3,W4,S
DOUBLE PRECISION TCRIT,PCRTT,ROCRIT,TOL,D41R
BWPSAT = ROKSL (T5)
BWPSAT = PCRTT - (((18502401000000. * S - 1254938500000.) *S +
1 34607546000.) *S - 629755380.) *S + 7312395.) *S** ( 3))
RETURN
END

$IBFTC BWROSV DECK
C SATURATED VAPOR DENSITY
DOUBLE PRECISION FUNCTION BWROSV(T8)
BWROSV = BWDENS(T8,BWPSAT(T8)-.00001)
RETURN
END

$IBFTC ROKSL DECK
C SATURATED LIQUID DENSITY INTERNAL UNITS GR-MOLE/CC
DOUBLE PRECISION FUNCTION ROKSL (T4)
COMMON/WORKS/WKS,W1,W2,W3,W4,S
COMMON/KONS/TCRIT,PCRTT,ROCRIT,TOL,D41R
DOUBLE PRECISION WKS,W1,W2,W3,W4,S
DOUBLE PRECISION TCRIT,PCRTT,ROCRIT,TOL,D41R
IF (T4.LT.TCRIT) GO TO 7
S=0.
GO TO 8
7 WKS= (TCRIT-T4)**(1./3.)
S = (((-.000020693181 * WKS -.00018306903) *WKS
1 +.0014973511) * WKS + .0062675345) *WKS
8 ROKSL= ROCRIT + S
RETURN
END

$IBFTC BWTSAT DECK
C SATURATION TEMPERATURE DEGREES KELVIN
DOUBLE PRECISION FUNCTION BWTSAT (P21)
BWTSAT=20.
W4= ALOG(P21)
DO 11 ITERS= 1,10
W3= BWTSAT + 1.0044
DELT = (W4 - (4.60659779 - 115.35279 / W3+ .0402605852*
1 BWTSAT ))/(115.35279 / W3**2 + .0402605852)
BWTSAT = BWTSAT + DELT
IF (DABS (DELT) - .0005) 3,3,11
11 CONTINUE

```

```

3 IF (BWT SAT .GE. 32.984) BWT SAT= 32.983
  RETURN
  END
$IBFTC DPDT DECK
C DPDT DERIVATIVE FOR THERMODYNAMIC GROUP REQUIRES BASIC MODULES
  DOUBLE PRECISION FUNCTION DPDT (T13)
  COMMON/WORKS/WKS,W1,W2,W3,W4,S
  COMMON/PTD/P,T,D,ROK,DELTA,XVAL
  COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
  COMMON/ACDEF/A(17)
  DOUBLE PRECISION WKS,W1,W2,W3,W4,S
  DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
  DOUBLE PRECISION A
  DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
  W1=EK*ROK
  W2=ROK**2
  DPDT= W2* (((-4.* (W1 * (A(15)*W2 + A(12))) + A(6))))
1 /T13 - 3.*W1 * (A(14)* W2 + A(11)))/T13 - 2.*
2 (W1 *(A(13) *W2 + A(10)) + A(5)))/T13
3 -A(4))/T13/T13 + A(1)/ROK + A(1) * A(2) +
4 ROK* (A(1) *A(7) + A(9)* ROK))
  RETURN
  END
$IBFTC BWTEMP DECK
C FUNCTION SUBROUTINE FOR TEMPERATURE IN C.G.S. UNITS
C AS FUNCTION OF DENSITY AND PRESSURE. REQUIRES BASIC GROUP
C USED FOR DENSITY CALCULATION
  DOUBLE PRECISION FUNCTION BWTEMP(DIN,P20)
  COMMON/PTD/P,T,D,ROK,DELTA,XVAL
  COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
  COMMON/ACDEF/A(17)
  COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
  COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
  DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
  DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
  DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
  DOUBLE PRECISION A
  DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
  D20= DIN
  T= TCRIT
  ROK= D20/2.01572
  WKS= ROK
  IF(P20-PCRIT) 10,13,13
13 CALL VAPOR
  XVAL= 2.
  CALL COEF(T)
  IF (PK(ROK) - P20) 55,11,11
10 T= BWT SAT(P20)
  CALL VAPOR
  IF(ROK-ROCRIT) 22,23,23
23 ROSL= ROKSL (T) * 2.01572
  IF (D20 - ROSL) 15,15,11
11 CALL LIQUID
  XVAL= -1.
  GO TO 55
22 ROSV= BWROSV (T)
  IF (ROSV - D20) 16,16,55
55 DO 67 I= 1,10
  ROK= WKS
  CALL COEF(T)

```

```

      EK=DEXP(-A(17)*ROK**2)
      DELTA= -(P20-PK(ROK))
      DELTA= DELTA/DPDT(T)
      T= T-DELTA
      IF(DABS(DELTA)- .0003) 77,77,67
67  CONTINUE
      GO TO 77
15  ROSV = BWROSV (T)
      GO TO 100
16  ROSL = ROKSL(T) * 2.01572
100 XVAL = (ROSL - D20)/ (ROSL - ROSV) * ROSV/D20
77  BWTEMP=T
      BWD= D20
      BWX=XVAL
      RETURN
      END
$IBFTC BWPRES  DECK
C      FUNCTION SUBROUTINE FOR PRESSURE IN C.G.S. UNITS
C      PRESSURE ATM AS FUNCTION OF TEMPERATURE AND DENSITY
C      REQUIRES BASIC MODULES USED FOR DENSITY CALCULATION
      DOUBLE PRECISION FUNCTION BWPRES(T17,D17)
      COMMON/ACOE/A
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
      DOUBLE PRECISION A
      DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      D17= DIN
      CALL VAPOR
      XVAL= 2.
      ROK= D17/2.0157
      IF(TCRIT-T17) 12,13,13
13  BWPRES= BWPSAT(T17)
      IF(ROK-ROCRIT) 17,14,14
14  ROSL = ROKSL (T17) * 2.01572
      IF (ROSL - D17) 11,72,72
11  CALL LIQUID
      XVAL= -1.
      GO TO 12
17  ROSV=BWROSV(T17)
      ROK=D17/2.0157
      IF(ROSV-D17)71,12,12
71  ROSL= ROKSL(T17) * 2.01572
      GO TO 100
72  ROSV= BWROSV (T17)
100 XVAL = (ROSL - D17) / (ROSL - ROSV)* ROSV / D17
      GO TO 77
12  CALL COEF(T17)
      BWPRES= PK(ROK)
77  BWX=XVAL
      BWD=D17
      RETURN
      END
$IBFTC PARALO  DECK
C      PARALO SUBROUTINE FOR IDEAL COEFFICIENTS, SPECIFIC HEAT OF
C      PARAHYDROGEN FOR TEMPERATURES LESS THAN 100 DEGREES KELVIN
      SUBROUTINE PARALO
      COMMON/CVS/CS,CH,F,E,U,C,B,AA

```

```

DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
AA = 4.977816011000 D0
B = -.3384077523 D-2
C = 3.521443735 D-4
U = -14.356331780-6
E = 23.03247505 D-8
F = -10.38316229 D-10
CH = .43 D0
CS = -.1984 D0
RETURN
END
$IBFTC PARAHI DECK
C      PARAHI SUBROUTINE FOR IDEAL SPECIFIC HEAT PARAHYDROGEN
C      COEFFICIENTS FOR TEMPERATURES ABOVE 100 DEGREES KELVIN
C      BUT LESS THAN 400 DEGREES KELVIN
      SUBROUTINE PARAHI
      COMMON/CSV/CS,CH,F,E,U,C,B,AA
      DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
      AA = -8.543812498 D0
      B = 29.35073908 D-2
      C = -19.64505888 D-4
      U = 6.145180979 D-6
      E = -.9172545570 D-8
      F = .05273284618 D-10
      CH = 432.3534 D0
      CS = 41.002 D0
      RETURN
      END
$IBFTC NORMLO DECK
C      NORMLO SUBROUTINES FOR IDEAL SPECIFIC HEAT NORMAL HYDROGEN
C      TEMPERATURES LESS THAN 100 DEGREES KELVIN
      SUBROUTINE NORMLO
      COMMON/CSV/CS,CH,F,E,U,C,B,AA
      DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
      AA = 4.960343508 D0
      B = .02245403779 D-2
      C = .4825909452 D-4
      U = -2.895260963 D-6
      E = 5.0980396 D-8
      F = -2.275937407 D-10
      CH = 254.03 D0
      CS = 4.151 D0
      RETURN
      END
$IBFTC NORMHI DECK
C      NORMHI SUBROUTINE FOR IDEAL COEFFICIENTS SPECIFIC HEAT OF
C      NORMAL HYDROGEN TEMPERATURES ABOVE 100 DEGREES KELVIN UP TO
C      400 DEGREES KELVIN
      SUBROUTINE NORMHI
      COMMON/CSV/CS,CH,F,E,U,C,B,AA
      DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
      AA = 3.809873570 D0
      B = 1.2237926310 D-2
      C = .8816230861 D-4
      U = -.6662777844 D-6
      E = .1533405461 D-8
      F = -.0121587109 D-10
      CH = 301.14435 D0
      CS = 8.11846885 D0
      RETURN

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      END
$IBFTC COEFID DECK
C      COEFID SUBROUTINE FOR SETTING UP IDEAL COEFFICIENTS
C      NORMAL OR PARA MODE
      SUBROUTINE COEFID (T1)
      COMMON/FIXED/MODE,ITERS
      IF(MODE-1) 1,1,2
      1 IF(T1-100.) 11,12,12
      11 CALL PARALO
      RETURN
      12 CALL PARAHI
      RETURN
      2 IF(T1-100.) 21,22,22
      21 CALL NORMLO
      RETURN
      22 CALL NORMHI
      RETURN
      END
$IBFTC BWCPIG DECK
C      FUNCTION SUBROUTINE FOR SPECIFIC HEAT IDEAL GAS NORMAL OR
C      PARAHYDROGEN ALL TEMPERATURES UP TO 400 DEGREES KELVIN
      DOUBLE PRECISION FUNCTION BWCPIG(T10)
      COMMON/CSV/CS,CH,F,E,U,C,B,AA
      DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
      CALL COEFID(T10)
      BWCPIG = 1./2.01572*(((F*T10+E)*T10+U)*T10+C)*T10+B)
      1 *T10+AA)
      RETURN
      END
$IBFTC BWHIDG DECK
C      FUNCTION SUBROUTINE FOR ENTHALPY IDEAL GAS T LESS THAN 400 DEG K
      DOUBLE PRECISION FUNCTION BWHIDG(T10)
      COMMON/CSV/CS,CH,F,E,U,C,B,AA
      DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
      CALL COEFID (T10)
      BWHIDG=1./2.01572*(CH+((((F/6.*T10+E/5.)*T10
      1 +U/4.)*T10+C/3.)*T10+B/2.)*T10+AA)*T10)
      RETURN
      END
$IBFTC BWSIDG DECK
      DOUBLE PRECISION FUNCTION BWSIDG(T10)
C      FUNCTION SUBROUTINE FOR ENTROPY IDEAL GAS T LESS THAN 400 DEG K
      COMMON/CSV/CS,CH,F,E,U,C,B,AA
      DOUBLE PRECISION CS,CH,F,E,U,C,B,AA
      CALL COEFID (T10)
      BWSIDG = 1./2.01572*(CS+AA*DLOG(T10)+((((F/5.*T10
      1 +E/4.)*T10+U/3.)*T10+C/2.)*T10+B)*T10)
      RETURN
      END
$IBFTC BWSSTL DECK
C      FUNCTION SUBROUTINE FOR ENTROPY SATURATED LIQUID PARAHYDROGEN
      DOUBLE PRECISION FUNCTION BWSSTL(T11)
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      BWSSTL = 1./2.01572*(5.77919623-2.*.43272654*
      1 (TCRIT-T11))*((1./2.) - 1.3333618*DLOG(T11)+
      2 ((.00017227638/3.*T11-.012869527/2.)*T11
      3 +.36251851)*T11)
      RETURN
      END

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$IBFTC BWHSTL DECK
C FUNCTION SUBROUTINE FOR ENTHALPY SATURATED LIQUID PARAHYDROGEN
DOUBLE PRECISION FUNCTION BWHSTL(T11)
COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
COMMON/WORKS/WKS,W1,W2,W3,W4,S
DOUBLE PRECISION WKS,W1,W2,W3,W4,S
DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
W = ROKSL(T11)
W = DLOG(W)*3.136424038+
1 S*1000.*((((2158613.45*S-190139.7999)*S
2 +7954.57119)*S-245.8927562)*S+6.72800008)*S
3 -.2054354458)
W = -120.142080*(W+13.073164)
BWHSTL = W+1./2.01572*(-53.43794-2.*.43272654
1 *(2.*TCRIT+T11)/3.*(TCRIT-T11)**(1./2.))
2 +((((0.00017227638/4.*T11-.012869527/3.)*T11
3 +.36251851/2.)*T11-1.3333618)*T11)
RETURN
END

$IBFTC BWSSV DECK
C FUNCTION SUBROUTINE FOR ENTROPY SATURATED VAPOR HYDROGEN
C EITHER PARA OR NORMAL AS A FUNCTION OF SATURATION PRESSURE
DOUBLE PRECISION FUNCTION BWSSV(P23)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
T= BWTSAT(P23)
ROK= 0
BWSSV= SKSV(P23)
D= ROK*2.01572
RETURN
END

$IBFTC SKSL DECK
C FUNCTION SATURATED LIQUID ENTROPY AS FUNCTION OF PRESSURE
DOUBLE PRECISION FUNCTION SKSL(P24)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
CALL LIQUID
SKSL= BWSSTL(T)
RETURN
END

$IBFTC BWSSL DECK
C ENTROPY SATURATED VAPOR INTERNAL UNITS REQUIRES BASIC AND
C THERMODYNAMIC MODULES
DOUBLE PRECISION FUNCTION BWSSL(P25)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
T= BWTSAT(P25)
BWSSL= SKSL(P25)
D= ROKSL(T)*2.01572
RETURN
END

$IBFTC HKSV DECK
C ENTHALPY SATURATED VAPOR PARA OR NORMAL HYDROGEN REQUIRES
C BASIC AND THERMO GROUP OF MODULES
DOUBLE PRECISION FUNCTION HKSV(P22)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
COMMON/WORKS/WKS,W1,W2,W3,W4,S
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R

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      DOUBLE PRECISION WKS,W1,W2,W3,W4,S
      DSV= BWRDSV(T)
12  HKSV= BWHIDG(T) + HDEV(T,ROK,P22)
      RETURN
      END
$IBFTC HKSL      DECK
      DOUBLE PRECISION FUNCTION HKSL(P24)
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
      CALL LIQUID
      HKSL= BWHSTL(T)
      RETURN
      END
$IBFTC SKSV      DECK
      DOUBLE PRECISION FUNCTION SKSV(P22)
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION WKS,W1,W2,W3,W4,S
      DSV= BWRDSV(T)
12  SKSV= BWSIDG(T)+SDEV(T,ROK,P22)
      SIDG= BWSIDG(T)
      RETURN
      END
$IBFTC HDEV      DECK
C      ENTHALPY DEVIATION TERM REQUIRES THERMO AND BASIC FUNCTIONS
      DOUBLE PRECISION FUNCTION HDEV(TD,RD,PD)
      COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
      COMMON/ACDEF/A(17)
      DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
      DOUBLE PRECISION A
      CK= (1.-EK)/2./A(17)
      C2= (CK-EK*RD*RD/2.)/A(17)
      HDEV= 1./2.01572/41.29283*(((A(16)/5.*RD**3+A(8)/2.)
1  *RD+((5.*A(6))/TD/TD+3.*A(5))/TD+2.*A(4))/TD+A(3))*RD
2  +1./TD/TD*(((5.*A(12))/TD+4.*A(11))/TD+3.*A(10))*CK
3  +((5.*A(15))/TD+4.*A(14))/TD+3.*A(13))*C2 )
4  +PD/RD-AF)
      RETURN
      END
$IBFTC BWHSV      DECK
      DOUBLE PRECISION FUNCTION BWHSV(P23)
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
      T= BWTSAT(P23)
      ROK= 0
      BWHSV= HKSV(P23)
      D= ROK*2.01572
      RETURN
      END
$IBFTC BWHSL      DECK
C      ENTHALPY SATURATED LIQUID INTERNAL UNITS REQUIRES BASIC AND
C      THERMO GROUP OF FUNCTIONS
      DOUBLE PRECISION FUNCTION BWHSL(P25)
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
      T= BWTSAT(P25)
      BWHSL= HKSL(P25)

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D= ROKSL(T)*2.01572
RETURN
END

$IBFTC SDEV DECK
C DEVIATION TERM FOR ENTROPY FUNCTION REQUIRES BASIC AND THERMO
DOUBLE PRECISION FUNCTION SDEV(TD,RD,PD)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
COMMON/ACOE/A(17)
DOUBLE PRECISION A
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
CK= (1.-EK)/2./A(17)
C2= (CK-EK*RD*RD /2.)/A(17)
SDEV= 1./2.01572/41.29283*(((A(9)/3.*RD-(A(7)*A(1))/2.)
1*RD-((-4.*A(6)/TD/TD-2.*A(5))/TD-A(4))/TD/TD
2-A(1)*A(2))*RD-A(1)*DLOG(RD*A(1)*TD)+
3(((4.*A(12)/TD+3.*A(11))/TD+2.*A(10))*CK+
4((4.*A(15)/TD+3.*A(14))/TD+2.*A(13))*C2)/TD/TD/TD)
RETURN
END

$IBFTC BWENHY DECK
C ENTHALPY OF PARA OR NORMAL HYDROGEN AS FUNCTION F TEMPERATURE
C AND PRESSURE IN C.G.S. UNITS REQUIRES BASIC AND THERMO GROUPS
DOUBLE PRECISION FUNCTION BWENHY(T12,P12)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
COMMON/WORKS/WKS,W1,W2,W3,W4,S
COMMON/ACOE/A(17)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION A
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION WKS,W1,W2,W3,W4,S
D= BWDENS(T12,P12)
BWENHY= HDEV(T12,ROK,P12)
IF(XVAL-2.) 1,2,2
2 BWENHY=BWENHY+ BWHIDG(T12)
RETURN
1 W4= ROKSL(T12)
EK= DEXP (-A(17)*W4*W4)
W3= HDEV(T12,W4,BWPSAT(T12))
PSA=BWPSAT(T12)
HL=BWHSTL(T12)
BWENHY= BWENHY+BWHSTL(T12)-W3
RETURN
END

$IBFTC BWERPY DECK
C ENTROPY OF PARA OR NORMAL HYDROGEN AS FUNCTION F TEMPERATURE
C AND PRESSURE IN C.G.S. UNITS REQUIRES BASIC AND THERMO GROUPS
C REQUIRES THERMODYNAMIC AND BASIC MODULES
DOUBLE PRECISION FUNCTION BWERPY(T12,P12)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
COMMON/WORKS/WKS,W1,W2,W3,W4,S
COMMON/ACOE/A(17)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION A
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION WKS,W1,W2,W3,W4,S
D= BWDENS(T12,P12)
BWERPY= SDEV(T12,ROK,P12)
IF(XVAL-2.) 1,2,2

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2 BWERPY= BWERPY+BWSIDG(T12)
RETURN
1 W4= ROKSL(T12)
EK= DEXP (-A(17)*W4*W4)
W3= SDEV(T12,W4,BWPSAT(T12))
BWERPY= BWERPY+BWSSTL(T12)-W3
RETURN
END
$IRFTC BWTOFH DECK
C SUBROUTINE FOR TEMPERATURE AS FUNCTION OF ENTHALPY AND PRESSURE
C IN C.G.S. UNITS FOR NORMAL OR PARAHYDROGEN REQUIRES BASIC
C AND THERMODYNAMIC MODULES
DOUBLE PRECISION FUNCTION BWTOFH(H23,P23)
COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
IF(P23-PCRIT)1,1,2
1 T=BWTSAT(P23)
ROK=0
HSV=HKSV(P23)
HSL=HKSL(P23)
IF (HSL - H23) 4,3,3
3 H=HSL
GOTO 11
4 IF (H23 - HSV) 8,8,9
8 BWTOFH = T
BWX= (H23 - HSL) / (HSV - HSL)
D= ROKSL(T)
BWD= 2.01572* (ROK* D) / (BWX* D + (1. - BWX) *ROK)
RETURN
2 T=33.0
H=BWENHY(33.0,P23)
IF (H23 - H) 29,29,19
9 H = HSV
GOTO 19
29 T=32.9
H=BWENHY (T,P23)
IF (H23 - H) 11,30,30
30 BWTOFH = TCRIT
RETURN
19 TNO = T
TN1 = TNO+10.
REG= 2.
TSP = TNO
GO TO 49
11 TNO = T
TN1 = TNO - 4.0
REG= -1.
TSP= TNO
49 FTO = H - H23
DO 77 ITER= 1,10
FT1= BWENHY (TN1,P23) - H23
DELTA = ((TN1 - TNO)* FT1) / (FT1 - FTO)
TN2 = TN1 - DELTA
IF (DABS(FTO) - DABS(FT1)) 71,72,72
72 TNO = TN1
FTO = FT1

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71 TN1 = TN2
   DELTA=DABS(TN2-TNO)
   IF (DELTA - .001 ) 76,77,77
77 CONTINUE
76 BWTOFH = TN2
   IF (ABS(REG-BWX) .LT. .001) GO TO 277
   IF (REG.LT.2.) GO TO 177
   BWD= BWROSV(TSP)
178 BWX= REG
   BWTOFH= TSP
277 RETURN
177 BWD= 2.01572* ROKSL(TSP)
   GO TO 178
END
$IBFTC BWTOFS DECK
C      SUBROUTINE FUNCTION FOR TEMPERATURE GIVEN ENTROPY AND PRESSURE
C      FOR NORMAL /OR PARAHYDROGEN IN C.G.S. UNITS REQUIRES BASIC AND
C      THERMODYNAMIC FUNCTIONS
      DOUBLE PRECISION FUNCTION BWTOFS(S23,P23)
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
      DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      IF(P23-PCRIT) 1,1,2
1  T= BWTSAT(P23)
   ROK= 0.
   SSV= SKSV(P23)
   SSL= SKSL(P23)
   IF(SSL-S23) 4,3,3
3  S= SSL
   GO TO 11
4  IF(S23-SSV) 8,8,9
8  BWTOFS= T
   BWX= (S23 - SSL) / (SSV-SSL)
   D= ROKSL(T)
   BWD= 2.01572* (ROK* D) / (BWX* D + (1. - BWX) *ROK)
   RETURN
2  T=33.0
   S=BWERPY(33.0,P23)
   IF(S23-S) 29,29,19
9  S= SSV
   GO TO 19
29 S=BWERPY(32.5,P23)
   IF(S23-S) 39,30,30
30 BWTOFS= TCRIT
   RETURN
39 T=32.5
   GO TO 11
19 TNO= T
   TN1= TNO+10.
   REG= 2.
   TSP= TNO
   GO TO 49
11 TNO= T
   TN1= TNO-4.0
   REG= -1.
   TSP= TNO
49 FTO= S-S23

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DO 77 ITER= 1,10
FT1= BWERPY(TN1,P23)-S23
DELTA= ((TN1-TN0)*FT1)/(FT1-FT0)
TN2= TN1-DELTA
IF(DABS(FT0)-DABS(FT1)) 71,72,72
72 TN0= TN1
FT0= FT1
71 TN1= TN2
DELTA=DABS(TN2-TN0)
IF (DELTA - .001 ) 76,77,77
77 CONTINUE
76 BWTOFS= TN2
IF (ABS(REG-BWX) .LT. .001) GO TO 277
IF (REG .LT.2.) GO TO 177
BWD= BWROSV(TSP)
178 BWX= REG
BWTOFS= TSP
277 RETURN
177 BWD= 2.01572* ROKSL(TSP)
GO TO 178
END

$IBFTC BWFD2 DECK
C SECOND-DERIVATIVE FUNCTION FOR SPECIFIC HEAT CALCULATION
C REQUIRES BASIC AND THERMODYNAMIC MODULES
DOUBLE PRECISION FUNCTION BWFD2(T24,R024)
COMMON/ACOFF/A(17)
COMMON/FTS/AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
DOUBLE PRECISION A
DOUBLE PRECISION AF,BF,CF,DF,EF,FF,B1,C1,C2,CK,E1,EK
EK= DEXP(-A(17)*R024**2)
BWFD2= 1./T24**3/83.238*((10.*A(6)/T24**2+3.*A(5)
1 +A(4)*T24)*2.*R024+
2 ((1.-EK)/A(17))*((10.*A(12)/T24+6.*A(11))/T24+3.*A(10)))+
3 ((1.-(A(17)*R024**2+1.)*EK)/A(17)**2)*
4 ((10.*A(15)/T24+6.*A(14))/T24+3.*A(13)))
RETURN
END

$IBFTC BWCPGL DECK
C SUBROUTINE FUNCTION FOR SPECIFIC HEAT CP AND CV
C ALSO CALCULATES SONIC VELOCITY CO FOR PARA OR NORMAL
C HYDROGEN IN C.G.S. UNITS REQUIRES BASIC AND THERMO MODULES
DOUBLE PRECISION FUNCTION BWCPGL(T25,P25)
COMMON/BWSONV/BWCO
COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION BWCO
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
D= BWDENS(T25,P25)
IF(XVAL-2.) 11,22,22
22 IF (T25.LE.46.) GO TO 10
23 BWCVGL= BWCPIG(T25) - .98584 -BWFD2(T25,ROK)
GO TO 66
10 IF (D.LT. .030774) GO TO 23
11 BWCVGL= BWFD2(T25,.037821)
BWCVGL= BWCVGL-BWFD2(T25,ROK)
IF(42.5-T25) 3,12,12
12 IF(24.5-T25) 2,1,1
1 BWCVGL=BWCVGL+((-0.11*T25+0.67)*T25+2.327)/8.4337
GO TO 66

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2 BWCVGL= BWCVGL+((-0.003*T25+0.302)*T25+6.554)/8.4337
GO TO 66
3 BWCVGL=BWCVGL+((.0002*T25+.0492)*T25+11.5398)/8.4337
66 WKS= DABS (PPK(ROK))
BWCPL= BWCVGL + T25 * DPDT(T25) **2 /ROK**2 / WKS / 83.238
BWCU= DABS(WKS * BWCPL / BWCVGL *502673.98)
BWCO= SQRT (BWCU)
RETURN
END

$IBFTC BWVISC DECK
C      VISCOSITY SUBROUTINE AS FUNCTION OF TEMPERATURE AND PRESSURE
C      FOR NORMAL OR PARAHYDROGEN ALSO CALCULATES CONDUCTIVITY K
C      REQUIRES BASIC AND THERMO GROUPS AND ALSO HIGH TEMPERATURE
DOUBLE PRECISION FUNCTION BWVISC(T15,P15)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION P,T,D,ROK,DELTA,XVAL
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
T400= 400.
IF(T15.GT.T400) GO TO 401
CPIG=BWCPIG(T15)
50 D= BWDENS(T15,P15)
GO TO 51
401 CPIG= HTCPIG(T15)
D= HTDENS(T15,P15)
51 CONTINUE
VI=0.8411* 1.D-4 *(.1017*T15**(3./2.)*
1 (T15 + 650.39))/(T15 + 19.55)/(T15+1175.9)
OVTERM= -58.75 * (D/.07)**3
IF (OVTERM.LT.-67.) OVTERM = -67.
DTERM= 5.7694 + 65. * D**(3./2.) -.000006*DEXP(127.2*D)
1 + 1./T15* (10.+ 7.2 *((D/.07)**6
2 -(D/.07)**(3./2.)) - 17.63 * DEXP (OVTERM))
BWVISC= 1.D4 * (VI + 1.D-6 *D *DEXP (DTERM))
BWCOND= 1.D4 *VI*((-T15*.004458+ 1.8341)/2.01572 +
1 (.0008973*T15 + 1.1308)*CPIG)/(1.+3.2/T15) +
2 1.D4* ((( (( (33615000.*D - 11243300.)*D + 1567680.)*D-
3 116927.)*D + 4952.28)*D - 115.024)*D+1.22648)*D +
4 .001102)*D+ .00000184)
RETURN
END

$IBFTC HTCPIG DECK
C      HIGH TEMPERATURE SPECIFIC HEAT FUNCTION 400 - 1500 DEG K
C      PARA OR NORMAL HYDROGEN
FUNCTION HTCPIG(T3)
COMMON/FIXED/MODE,ITERS
IF(1-MODE) 1,2,2
1 IF(700.1-T3) 2,3,3
3 HTCPIG= (.0000001071*T3-.0000221)*T3+3.4528
RETURN
2 IF(T3-700.) 4,4,5
4 HTCPIG= 1./2.01572*((.000001*T3-.001005)*T3+7.25125)
RETURN
5 HTCPIG= 1./2.01572*((.0000005*T3-.0002458)*T3+6.96481)
RETURN
END

$IBFTC HTHIDG DECK
C      HIGH TEMPERATURE ENTHALPY IDEAL GAS ABOVE 400 DEG K
FUNCTION HTHIDG(T3)
COMMON/FIXED/MODE,ITERS

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      IF(T3-700.) 11,11,21
11 HTHIDG= 1./2.01572*((.000001/3.*T3-.001005/2.)*T3
   1 +7.25125)*T3-112.2412)
      RETURN
21 HTHIDG= 1./2.01572*((.0000005/3.*T3-.0002458/2.)*T3
   1 +6.96481)*T3-40.5934)
      RETURN
      END
$IBFTC HTSIDG DECK
C      HIGH TEMPERATURE ENTROPY IDEAL GAS ABOVE 400 DEG K
      FUNCTION HTSIDG(T3)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      IF(1-MODE) 1,1,2
   1 HTSIDG= -4.903 + 2.76/2.01572
      GO TO 3
   2 HTSIDG= -4.903
   3 IF (T3-700.) 4,4,5
   4 HTSIDG= HTSIDG+ 1./2.01572*(7.25125*ALOG(T3)
   1 +(.000001/2.*T3-.001005)*T3)
      GO TO 6
   5 HTSIDG= HTSIDG+.680+ 1./2.01572*(6.96481*ALOG(T3)+(.0000005/2.
   1 *T3-.0002458)*T3)
   6 RETURN
      END
$IBFTC HTHDEV DECK
C      THERMAL DEVIATION TERM FOR ENTHALPY FUNCTION ABOVE 400 DEG K
      FUNCTION HTHDEV(TD,RD,PD)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      BP= W4/TD*((1.25*.22004*W2+.75*.036877)*W2-.25*.0055478)*W3
      CP= W2/TD**2*W2*(2.*.04053*W2-1.5*.004788)*W3**2
      F1= BT**2
      D1= BT
      D2= F1/2.+CT
      D3= BT*F1/6.+BT*CT
      D4= F1**2/24.+F1*CT/2.+(CT**2)/2.
      F1= BP
      F2= (BP*D1+CP)/2.
      F3= (BP*D2+CP*D1)/3.
      F4= (BP*D3+CP*D2)/4.
      F5= (BP*D4+CP*D3)/5.
      F6= (CP*D4)/6.
      HTHDEV= 1./41.29283*(-82.082/2.01572*TD*TD*
   1 (((((F6*ROK+F5)*ROK+F4)*ROK+F3)*ROK
   2 +F2)*ROK+F1)*ROK)+PD/ROK-82.082/2.01572*TD)
      RETURN
      END
$IBFTC HTENHY DECK
C      ENTHALPY OF PARA OR NORMAL HYDROGEN TEMPERATURES ABOVE 400 DEG K

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C      REQUIRES HIGH TEMPERATURES MODULES
      FUNCTION HTENHY(T2,P2)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      D= HTDENS(T2,P2)
      HTENHY= HTHDEV(T2,ROK,P2)+HTHIDG(T2)
      RETURN
      END
$IBFTC HTSDEV DECK
C      ENTROPY THERMAL DEVIATION FOR HIGH TEMPERATURE FUNCTION
      FUNCTION HTSDEV(TD,RO,PD)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      BP= W4/TD*((1.25*.22004*W2+.75*.036877)*W2-.25*.0055478)*W3
      CP= W2/TD**2*W2*(2.*.04053*W2-1.5*.004788)*W3**2
      F1= BT**2
      D1= BT
      D2= F1/2.+CT
      D3= BT*F1/6.+BT*CT
      D4= F1**2/24.+F1*CT/2.+(CT**2)/2.
      F1= BP
      F2= (BP*D1+CP)/2.
      F3= (BP*D2+CP*D1)/3.
      F4= (BP*D3+CP*D2)/4.
      F5= (BP*D4+CP*D3)/5.
      F6= (CP*D4)/6.
      HTSDEV= -D41R*(((D4/4.*ROK+D3/3.)*ROK+D2/2.)*ROK
1 +D1)*ROK
2 +TD*(((F6*ROK+F5)*ROK+F4)*ROK+F3)*ROK
3 +F2)*ROK+F1)*ROK)
4+ALOG(ROK*D41R*TD))/41.29243
      RETURN
      END
$IBFTC HTERPY DECK
C      ENTROPY OF PARA OR NORMAL HYDROGEN FOR TEMPERATURES ABOVE
C      400 DEG K REQUIRES HIGH TEMPERATURE MODULES
      FUNCTION HTERPY(T2,P2)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      D= HTDENS(T2,P2)
      HTERPY= HTSDEV(T2,ROK,P2)+HTSIDG(T2)
      RETURN
      END
$IBFTC HTIOPS DECK
C      TEMPERATURE AS FUNCTION OF ENTHALPY AND PRESSURE

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C      FOR PARA OR NORMAL HYDROGEN IN REGION ABOVE 400 DEG K
      FUNCTION HTTOFS(S5,P5)
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      T=400.
      DO 77 I=1,10
      S=HTERPY(T,P5)
      CVGL=HTCPIG(T)-.9854-1.98646/82.082*HTFD2(T,ROK)
      D= (CVGL+T*(HTDPDT(T)/ROK)**2/PP/82.0821*1.98646)/T
      DELTA= (S-S5)/D
      T=T-DELTA
      IF(ABS(DELTA)-.01) 2,2,77
77 CONTINUE
      HTTOFS=T
      RETURN
      END
$IRFTC HTDPDT DECK
C      DERIVATIVE DPDT FOR HIGH TEMPERATURE REGION FUNCTIONS
      FUNCTION HTDPDT(TD)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      BP= 1./TD*W4*((1.25*.22004*W2+.75*.036877)*W2
1 -.25*.0055478)*W3
      CP= 1./TD**2*W2*(2*.04053*W2-1.5*.004788)*W3**2
      HTDPDT= D41R*ROK*(ROK*TD*(BP+CP*ROK)+1.)*EXPF
      RETURN
      END
$IRFTC HTDENS DECK
C      DENSITY FUNCTION GIVEN TEMPERATURE AND PRESSURE IN C.G.S. UNITS
C      FOR HIGH TEMPERATURE PARA OR NORMAL HYDROGEN
      FUNCTION HTDENS(T1,P1)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      D41R= 82.082/2.01572
      ROK= P1/T1/D41R
      W2=1./T1*(1./2.)
      W4= W2*(1./2.)
      W3= 1000./0.089888
      RT= W4*(.0055478+W2*(-.22004*W2-.036877))*W3
      CT= 1./T1*W2*(-.04053*W2+.0047880)*W3**2
      DO 1 I=1,10
      EXPF= EXP((CT*ROK+BT)*ROK)
      P= D41R*T1*ROK*EXPF
      PP= D41R*T1*EXPF*(ROK*(BT+2.*CT*ROK)+1.)
      DELTA= (P-P1)/PP
      ROK= ROK-DELTA
      IF(ABS(DELTA)-.0000005) 70,70,1
1 CONTINUE
70 D=ROK

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        HTDENS= D
        BWD= D
        BWX= 2.
        RETURN
    END
$IBFTC HTFD2 DECK
C      SECOND DERIVATIVE FUNCTION FOR SPECIFIC HEAT CALCULATION
      FUNCTION HTFD2(T9,R9)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXP
      COMMON/WORKS/WKS,W1,W2,W3,W4,S
      COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
      DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
      BPP= 1./16./T9/T9*W4*((-45.*.22004*W2
1 -21.*.036877)*W2+5.*.0055478)*W3
      CPP= 1./T9**3*(-6.*.04053*W2+3.75*.004788)*W2*W3*W3
      A0= 2.*BPP+T9*BPP
      A1= BP**2+2.*CP+T9*CPP
      A2= 2.*T9*BP*CP
      A3= T9*CP**2
      G1= A0
      G2= (A0*D1+A1)/2.
      G3= (A0*D2+A1*D1+A2)/3.
      G4= (A0*D3+A1*D2+A2*D1+A3)/4.
      G5= (A0*D4+A1*D3+A2*D2+A3*D1)/5.
      G6= (A1*D4+A2*D3+A3*D2)/6.
      G7= (A2*D4+A3*D3)/7.
      G8= (A3*D4)/8.
      HTFD2= 82.082/2.01572*T9*(((((((G8*R9+G7)*R9+G6)
2 *R9+G5)*R9+G4)*R9+G3)*R9+G2)*R9+G1)*R9)
      RETURN
    END
$IBFTC HTTOFH DECK
C      TEMPERATURE AS A FUNCTION OF ENTHALPY AND PRESSURE FOR
C      PARA OR NORMAL HYDROGEN ABOVE 400 DEGREES KELVIN
      FUNCTION HTTOFH(H5,P5)
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL
      COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXP
      T= 400.
      DO 77 I= 1,10
      H=HTENHY(T,P5)
      BWCVGL= HTCPGL(T)-.9854-1.98646/82.082*HTFD2(T,ROK)
      D= BWCVGL+T*(HTDPDT(T)/ROK)**2/PP/82.0821*1.98646
      DELTA= (H-H5)/D
      T= T-DELTA
      IF(ABS(DELTA)-.01) 2,2,77
77 CONTINUE
2 HTTOFH= T
      RETURN
    END
$IBFTC HTCPGL DECK
C      SPECIFIC HEAT OF NORMAL OR PARA HYDROGEN AS FUNCTION
C      OF TEMPERATURE AND PRESSURE IN C.G.S. UNITS ABOVE 400 DEG K
      FUNCTION HTCPGL(T4,P4)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
      COMMON/PTD/P,T,D,ROK,DELTA,XVAL

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COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
COMMON/WORKS/WKS,W1,W2,W3,W4,S
COMMON/KONS/TCRIT,PCRIT,ROCRIT,TOL,D41R
DOUBLE PRECISION BWCO
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION TCRIT,PCRIT,ROCRIT,TOL,D41R
D= HTDENS(T4,P4)
BWCVGL= HTPIG(T4)-.9854-1.98646/82.082*HTF02(T4,ROK)
HTCPGL= BWCVGL+T4*(HTDPDT(T4)/ROK)**2
1 /PP/82.082*1.98646
BWCO = SQRT( PP * HTCPGL/BWCVGL * 502673.98* 2.01572)
RETURN
END

$IBFTC HTEMP DECK
FUNCTION HTEMP(DIN,P20)
COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
ROK=DIN
T=400.
XVAL=2.
DO 67 I=1,10
DELTA = -(P20 - HTPRES(T,ROK))
DELTA = DELTA / HTDPDT(T)
T=T - DELTA
IF (ABS(DELTA) - .0003 ) 77,77,67
67 CONTINUE
GO TO 77
77 HTEMP = T
BWD=DIN
BWX= XVAL
RETURN
END

$IBFTC HTPKS DECK
FUNCTION HTPRES(T1,DD)
COMMON/PTD/P,T,D,ROK,DELTA,XVAL
COMMON/PVS/PP,BT,CT,BP,CP,H,D1,D2,D3,D4,EXPF
D41R= 82.082/2.01572
ROK=DD
W2=SQRT(1./T1)
W4=SQRT(W2)
W3=1000./-.089888
BT=W4*(.0055478 +W2 *(-.22004*W2 - .036877))*W3
CT= 1./T1*W2*(-.04053*W2 + .004788)*W3**2
EXPF= EXP((CT*ROK + BT) *ROK)
HTPRES= D41R * T1 * ROK * EXPF
RETURN
END

$IBFTC BT DECK
C FUNCTION SUBROUTINE REQUIRES FOR BRITISH THERMAL UNITS
C PARA OR NORMAL COMPOSITION ALL PROPERTIES N = 1 - 22 PARA
C AND N= 201 - 222 NORMAL HYDROGEN. PRESSURES PSI, AND
C TEMPERATURES DEGREES RANKIN
FUNCTION BT(N,P1,P2)
COMMON/FIXED/MODE,ITERS
COMMON/BWSONV/BWCO
COMMON/BTDXCK/BTD,BTX,BTCVGL,BTCOND,BTCO
COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION BTD,BTX,BTCVGL,BTCOND,BTCO

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DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION BWCO
MODE = N/100
T400= 400.*1.8
M= N - 100*MODE
BT= P1 + P2
IF (NTAG(BT).NE.0) GO TO 333
BWD=BT / 62.427
GOTO (1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22),M
333 BT= BT
BTX= BT
IF (M.NE.6) GO TO 334
BT= BT
BTX= BT
BTX= BT
RETURN
334 IF (M.NE.7) GO TO 335
BT= BT
BTX= BT
335 RETURN
1 IF (P1.GT.T400) GO TO 101
BT= 62.427 * BWDENS (P1/1.8, P2/14.696)
GO TO 77
101 BT= 62.427 * HTDENS (P1/1.8,P2/14.696)
GO TO 77
2 IF (P1.GT.T400) GO TO 102
BT= 1.79882 * BWENHY(P1/1.8, P2/14.696)
GO TO 77
102 BT= 1.79882 * HTENHY (P1/1.8, P2/14.696)
GO TO 77
3 IF (P1.GT.T400) GO TO 103
BT= .99983 * BWERPY (P1/1.8, P2/14.696)
GO TO 77
103 BT= .99983 * HTERPY (P1/1.8, P2/14.696)
GO TO 77
4 H= 1.79882 * BWENHY (400. , P2/14.696)
IF (P1.GT.H) GO TO 104
BT= 1.8 * BWTOFH (P1/1.79882, P2/14.696)
GO TO 77
104 BT= 1.8 * HTTOFH (P1/1.79882, P2/14.696)
GO TO 77
5 S= .99983 * BWERPY(400.,P2/14.696)
IF (P1.GT.S) GO TO 105
BT= 1.8 * BWTOFS(P1/.99983, P2/14.696 )
GO TO 77
105 BT= 1.8 * HTTOFS (P1/.99983,P2/14.696)
GO TO 77
6 IF (P1.GT.T400) GO TO 106
BT= .99983 * BWCPGL (P1/1.8, P2/14.696)
BT= BT * BWCVGL*.99983
BTX= BTX / 2.54/12.
GO TO 77
106 BT= .99983 * HTCPGL (P1/1.8, P2/14.696)
BT= BT * BWCVGL*.99983
BTX= BTX / 2.54/12.
GO TO 77
7 BT= 1./14.882 * BWVISC (P1/1.8, P2/14.696)
BTX= BTX * BWCOND * .067163
GO TO 77
8 IF (P1.GT.T400) GO TO 108
BT= 14.696 * BWPRES(P1/1.8,P2/62.427)
GO TO 77

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108 HT=14.696 * HTPRES(P1/1.8, P2/62.427)
   GO TO 77
   9 P=BWPRES(T400,P1/62.427)
   IF (P2/14.696 .GT. P) GO TO 109
   RT= 1.8 * BWTEMP(P1/62.427,P2/14.696)
   GO TO 77
109 HT=1.8 * HTTEMP (P1/62.427, P2/14.696)
   GO TO 77
10 HT= 14.696 * BWPSAT (P1/1.8)
   GO TO 77
11 HT= 1.8 * BWTSAT (P1/14.696)
   GO TO 77
12 BT= 62.427 * 2.01572 * RUKSL (P1/1.8)
   GO TO 77
13 HT= 62.427 * BWROSV (P1/1.8)
   GO TO 77
14 IF (P1.GT.T400) GO TO 114
   RT= .99983 * BWCPIG (P1/1.8)
   GO TO 77
114 BT= .99983 * HTCPIG (P1/1.8)
   GO TO 77
15 PSAT = BWPSAT (P1 / 1.8) + .001
   RT= .99983 * BWCPGL (P1 / 1.8, PSAT)
   GO TO 77
16 PSAT= BWPSAT (P1/1.8) -.001
   RT= .99983 * BWCPGL (P1 / 1.8, PSAT)
   HTCVGL= HWCVGL*.99983
   GO TO 77
17 IF (P1.GT.T400) GO TO 117
   RT= 1.79882 * BWHIDG (P1/1.8)
   GO TO 77
117 BT= 1.79882 * HTHIDG (P1/1.8)
   GO TO 77
18 BT= 1.79882 * BWHSTL (P1 / 1.8)
   GO TO 77
19 PSAT = BWPSAT (P1 / 1.8) + .001
   RT= 1.79882 * BWHSV (PSAT)
   GO TO 77
20 IF (P1.GT.T400) GO TO 120
   RT= .99983 * BWSIDG (P1 / 1.8)
   GO TO 77
120 RT= .99983 * HTSIDG (P1/1.8)
   GO TO 77
21 BT= .99983 * BWSSTL (P1/1.8)
   GO TO 77
22 PSAT = BWPSAT (P1 / 1.8)
   RT= .99983 * BWSSV (PSAT)
77 BTD= BWD * 62.427
   BTX= BWX
   RETURN
   END
$IBFTC BI      DECK
C      BI FUNCTION USED FOR SYSTEM INTERNATIONAL UNITS
C      PARA OR NORMAL COMPOSITION ALL PROPERTIES N=1 - 22 PARA
C      AND N=201 - 222 NORMAL HYDROGEN.  PRESSURES NEWTON/SQ METER
C      AND TEMPERATURES DEGREES KELVIN
      FUNCTION BI(N,P1,P2)
      COMMON/FIXED/MODE,ITERS
      COMMON/BWSONV/BWCO
      COMMON/BIDXCK/BID,BIX,BICVGL,BICOND,BICO

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COMMON/BWDXCK/BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION BID,BIX,BICVGL,BICOND,BICO
DOUBLE PRECISION BWD,BWX,BWCVGL,BWCOND
DOUBLE PRECISION BWCO
MODE = N / 100
T400 = 400.
M = N - 100*MODE
BI = P1 + P2
IF (NTAG(BI) .NE. 0) GO TO 333
BWD = BID / 1000.
GO TO (1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22),M
333 BID = BI
BIX = BI
IF (M.NE.6) GO TO 334
BICVGL = BI
BICO = BI
RETURN
334 IF (M.NE.7) GO TO 335
BICOND = BI
335 RETURN
1 IF (P1.GT.T400) GO TO 101
BI = 1000. * BWDENS (P1,P2/101325.)
GO TO 77
101 BI = 1000. * HTDENS (P1,P2/101325.)
GO TO 77
2 IF (P1.GT.T400) GO TO 102
BI = 4184. * BWENHY(P1,P2/101325.)
GO TO 77
102 BI = 4184. * HTENHY(P1,P2/101325.)
GO TO 77
3 IF (P1.GT.T400) GO TO 103
BI = 4184. * BWERPY (P1,P2/101325.)
GO TO 77
103 BI = 4184. * HTERPY (P1,P2/101325.)
GO TO 77
4 H = 4184. * BWENHY(400.,P2/101325.)
IF (P1.GT.H) GO TO 104
BI = BWTOFH (P1/4184., P2/101325.)
GO TO 77
104 BI = HTTOFH(P1/4184.,P2/101325.)
GO TO 77
5 S = 4184. * BWERPY ( 400.,P2/101325.)
IF (P1.GT.S) GO TO 105
BI = BWTOFS(P1/4184.,P2/101325.)
GO TO 77
105 BI = HTTOFS(P1/4184.,P2/101325.)
GO TO 77
6 IF (P1.GT.T400) GO TO 106
BI = 4184. * BWCPGL (P1,P2/101325.)
BICVGL = BWCVGL * 4184.
BICO = BWCO / 100.
GO TO 77
106 BI = 4184. * HTCPGL (P1,P2/101325.)
BICVGL = BWCVGL * 4184.
BICO = BWCO / 100.
GO TO 77
7 BI = .1 * BWVISC (P1,P2/101325.)
BICOND = BWCOND * 418.4
GO TO 77
8 IF (P1.GT.T400) GO TO 108

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      BI = 101325. * BWPRES(P1,P2/1000.)
      GO TO 77
108 BI = 101325.* HTPRES(P1,P2/1000.)
      GO TO 77
      9 P = BWPRES(T400,P1/1000.)
      IF (P2/101325..GT.P) GO TO 109
      BI = BWTEMP (P1/1000.,P2/101325.)
      GO TO 77
109 BI = HTTEMP(P1/1000.,P2/101325.)
      GO TO 77
10 BI = 101325. * BWPSAT(P1)
      GO TO 77
11 BI = BWTSAT(P1/101325.)
      GO TO 77
12 BI = 1000. * 2.01572 * ROKSL(P1)
      GO TO 77
13 BI = 1000. * BWROSV(P1)
      GO TO 77
14 IF (P1.GT.T400) GO TO 114
      BI = 4184.*BWCPIG (P1)
      GO TO 77
114 BI = 4184. * HTCPIG(P1)
      GO TO 77
15 PSAT = BWPSAT (P1) + .001
      BI = 4184. * BWCPLG(P1,PSAT)
      BICVGL = 4184.* BWCVGL
      GO TO 77
16 PSAT = BWPSAT (P1)- .001
      BI = 4184. * BWCPLG(P1,PSAT)
      BICVGL = 4184.*BWCVGL
      GO TO 77
17 IF (P1.GT.T400) GO TO 117
      BI = 4184.* BWHIDG(P1)
      GO TO 77
117 BI = 4184. * HTHIDG(P1)
      GO TO 77
18 BI = 4184. * BWHSTL(P1)
      GO TO 77
19 PSAT = BWPSAT (P1) + .001
      BI = 4184.* BWHSV(PSAT)
      GO TO 77
20 IF (P1.GT.T400) GO TO 120
      BI = 4184.* BWSIDG(P1)
      GO TO 77
120 BI = 4184. * HTSIDG(P1)
      GO TO 77
21 BI = 4184.* BWSSTL(P1)
      GO TO 77
22 PSAT = BWPSAT (P1)
      BI = 4184.* BWSSV(PSAT)
77 BID = BWD * 1000.
      BIX = BWX
      RETURN
      END
$IBFTC NTAGS DECK
      FUNCTION NTAG(BWS)
      NTAG=0
      RETURN
      END

```

APPENDIX C

DERIVATIONS OF THERMODYNAMIC AND TRANSPORT EQUATIONS

Equations

In calculating thermodynamic functions such as enthalpy H and entropy S , or specific heats C_v or C_p , at either constant volume or pressure, it is desirable to avoid tabular interpolation or curve-fitting each function in two dimensions, but rather to relate these functions to the equation of state. To do this requires only that the equation of state be differentiable and integrable in the domain of interest. Furthermore, if these operations can be performed in closed form, the amount of necessary calculation may be greatly reduced. The following derivations demonstrate how to relate H and S to the equation of state.

In general, any state parameter is determined from the specification of any two other parameters. Therefore, if S is expressed as $S(\rho, T)$, entropy can then be formally written as

$$dS = \left(\frac{\partial S}{\partial T} \right)_{\rho} dT + \left(\frac{\partial S}{\partial \rho} \right)_T d\rho$$

From Maxwell's equation,

$$\left(\frac{\partial S}{\partial V} \right)_T = \left(\frac{\partial P}{\partial T} \right)_V$$

and

$$\rho = \frac{1}{V} : \left(\frac{\partial S}{\partial \rho} \right)_T = \frac{-1}{\rho^2} \left(\frac{\partial S}{\partial V} \right)_T = \frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_\rho$$

Hence,

$$dS = \left(\frac{\partial S}{\partial T} \right)_{\rho} dT - \frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} d\rho$$

From the second law of thermodynamics, $dH = T dS + (dP/\rho)$. Setting dP/ρ equal to $d(P/\rho) + P/\rho^2 d\rho$ yields

$$dH = T \left(\frac{\partial S}{\partial T} \right)_{\rho} dT + d \left(\frac{P}{\rho} \right) + \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

Note that along an isotherm the difference between the enthalpy or entropy, H and S , at density ρ , and the values of H_0 and S_0 at an arbitrary ρ_0 is

$$(H_{\rho} - H_{\rho_0})_T = \frac{P(T, \rho)}{\rho} - \frac{P(T, \rho_0)}{\rho_0} + \int_{\rho_0}^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

and

$$(S_{\rho} - S_{\rho_0})_T = \int_{\rho_0}^{\rho} \left[\frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

To avoid the difficulties inherent in integrating through the vapor dome, the problem can be subdivided into finding appropriate values of ρ_0 and corresponding expressions for $H_{\rho, T}$ and $S_{\rho, T}$ in the vapor region and in the compressed liquid region.

In the vapor region, the problem may be simplified further by calculating

$$(H_{\rho} - H_{\rho, id})_T \text{ and } (S_{\rho} - S_{\rho, id})_T.$$

Since P is equal to ρRT for an ideal gas,

$$(H_{\rho, id} - H_{\rho, o, id})_T = RT - RT + \int_{\rho_0}^{\rho} \left(\frac{P}{\rho^2} - \frac{P}{\rho^2} \right)_T d\rho = 0$$

$$(H_{\rho} - H_{\rho, id})_T - (H_{\rho, o} - H_{\rho, o, id})_T = \frac{P(T, \rho)}{\rho} - \frac{P(T, \rho_0)}{\rho_0} + \int_{\rho_0}^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

Since it is desirable, as the limit $\rho_0 \rightarrow 0$, that the properties of the real gas merge with those of the ideal gas and since calculating procedures demand that this be true, it is justifiable to use the following relation:

$$\lim_{\rho \rightarrow 0} (H - H_{id})_{\rho, T} = \frac{P(T, \rho)}{\rho} - RT + \int_0^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

If H_{id} is then expressed as a function of temperature only and, in the usual manner, is set equal to $H_{id}(T_0) + \int_{T_0}^T C_p(T) dT$, the following expression is obtained for H in the vapor region:

$$H(\rho, T) = H_{id}(T_0) + \int_{T_0}^T C_p(T) dT + \frac{P}{\rho} - RT + \int_0^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho$$

The ideal gas entropy deviation at constant temperature is

$$(S_{\rho, id} - S_{\rho, o, id})_T = \left[\int_{\rho, o, id}^{\rho, id} \frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} d\rho \right]_T = \int_{\rho, o, id}^{\rho, id} \left(\frac{-R}{\rho} \right)_T d\rho$$

or

$$(S_{\rho} - S_{\rho, id})_T - (S_{\rho, o} - S_{\rho, o, id})_T = \int_{\rho_o}^{\rho} \left[\frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho + \int_{\rho, o, id}^{\rho, id} \left(\frac{R}{\rho} \right)_T d\rho$$

In the limit as density approaches zero, one can arbitrarily set

$$\lim (S_{\rho, o} - S_{\rho, o, id}) = 0$$

Thus,

$$(S - S_{id})_{\rho, T} = \int_0^{\rho} \left[\frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right] d\rho + \int_0^{\rho, id} \left(\frac{R}{\rho} \right)_T d\rho$$

Since

$$\int_0^{\rho, \text{id}} \left(\frac{R}{\rho} \right)_T d\rho = \int_0^{\rho} \left(\frac{R}{\rho} \right)_T d\rho - \int_{\rho, \text{id}}^{\rho} \left(\frac{R}{\rho} \right)_T d\rho$$

and

$$\int_{\rho, \text{id}}^{\rho} \left(\frac{R}{\rho} \right)_T d\rho = R \ln \frac{\rho}{\rho_{\text{id}}}$$

where $\rho_{\text{id}} = P/RT$. Hence,

$$\int_{\rho, \text{id}}^{\rho} \left(\frac{R}{\rho} \right)_T d\rho = R \ln \frac{\rho RT}{P} = R \ln \frac{1}{Z}$$

Therefore,

$$(S - S_{\text{id}})_{\rho, T} = \int_0^{\rho} \left[\frac{R}{\rho} - \frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right) \right]_T d\rho - R \ln \frac{1}{Z}$$

If S_{id} is then expressed as equal to $S_{\text{id}}(T_0) + \int_{T_0}^T C_p(T)/T(T) dT - R \ln P$ where

$S_{\text{id}}(T_0)$ is the ideal gas entropy at 1 atmosphere ($1.01325 \times 10^5 \text{ N/m}^2$); $S_{T, \rho}$ in the vapor region is given by the expression

$$S_{T, \rho} = S_{\text{id}}(T_0) + \int_{T_0}^T \frac{C_p(T)}{T} dT - R \ln \frac{P}{Z} + \int_0^{\rho} \left[\frac{R}{\rho} - \frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right) \right]_T d\rho$$

In the compressed liquid region, the calculation of enthalpy and entropy can be simplified by letting ρ_0 be equal to the saturated liquid density for the given temperature. With that condition, the enthalpy and entropy differences may be expressed as

$$H(\rho, T) - H_{sl}(T) = \frac{P}{\rho} - \frac{P_{sat}(T)}{\rho_{sl}} + \int_{\rho_{sl}}^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho$$

and

$$S(\rho, T) - S_{sl}(T) = \int_{\rho_{sl}}^{\rho} \left[\frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho$$

To calculate $H_{\rho_{sat liq}}$ and $S_{\rho_{sat liq}}$, use can be made of the following properties:

$$H_{sl}(T) - H_{sv}(T) = P_{sat}(T) \left(\frac{1}{\rho_{sl}} - \frac{1}{\rho_{sv}} \right) + \int_{\rho_{sv}}^{\rho_{sl}} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho$$

Since the saturation pressure is not a function of density variation in the interval under the vapor dome,

$$dP \equiv \left(\frac{\partial P}{\partial T} \right)_{\rho} dT + \left(\frac{\partial P}{\partial \rho} \right)_{\rho} d\rho = \left(\frac{\partial P}{\partial T} \right)_{\rho} dT$$

Therefore,

$$\int_{\rho_{sv}}^{\rho_{sl}} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho = P_{sat}(T) \left(\frac{1}{\rho_{sv}} - \frac{1}{\rho_{sl}} \right) + T \left(\frac{dP_{sat}}{dT} \right) \left(\frac{1}{\rho_{sl}} - \frac{1}{\rho_{sv}} \right)$$

Hence,

$$H_{sl}(T) - H_{sv}(T) = T \left(\frac{dP_{sat}}{dT} \right) \left(\frac{1}{\rho_{sl}} - \frac{1}{\rho_{sv}} \right)$$

For entropy,

$$S_{sl}(T) - S_{sv}(T) = \int_{\rho_{sv}}^{\rho_{sl}} \left[\frac{-1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho} \right]_{\rho} d\rho$$

From these arguments, it is evident that

$$S_{sl}(T) - S_{sv}(T) = \frac{dP_{sat}}{dT} \left(\frac{1}{\rho_{sl}} - \frac{1}{\rho_{sv}} \right)$$

Since both $H_{sv}(T)$ and $S_{sv}(T)$ can be calculated as deviations from ideal gas conditions, the calculation of $H_{sl}(T)$ and $S_{sl}(T)$ would be relatively straightforward.

The calculations of $H_{sl}(T)$ and $S_{sl}(T)$ can be simplified further by considering the specific heat of the saturated liquid $C_{sl}(T)$. For parahydrogen this specific heat has been calculated and can be expressed as a function of temperature. Since this function is integrable in closed form, the change in entropy along the saturated liquid line may be expressed as

$$S_{sl}(T) = \int_{T_0}^T \frac{C_{sl}(T)}{T} dT + S_{sl}(T_0)$$

where $S_{sl}(T_0)$ is the entropy of the saturated liquid at temperature T_0 . Since from the second law of thermodynamics,

$$dH = T dS + \frac{dP}{\rho}$$

$$H_{sl}(T) = \int_{T_0}^T C_{sl}(T) dT + H_{sl}(T_0) + \int_{\rho_{sl}(T_0)}^{\rho_{sl}(T)} \frac{dP}{\rho}$$

where $H_{sl}(T_0)$ is the enthalpy of the saturated liquid at T_0 and $\int_{\rho_{sl}(T_0)}^{\rho_{sl}(T)} dP/\rho$ may be calculated from the saturation boundary equations.

Transport Properties

The calculation of real gas values of viscosity and thermal conductivity coefficients is complicated by the incompleteness of both theory and data. For ideal gas conditions, these coefficients are calculated from either theoretical relations (refs. 9 and 10) or empirical correlations (refs. 5 and 7).

Attempts have been made to apply real gas corrections by theoretical approaches such as that of Enskog (refs. 5 and 11). This approach relates functions of the state equation to concepts such as thermal motion and intermolecular forces necessary to describe transport properties. The method has met with little success, except at relatively low densities.

Graphical correlations (refs. 9 and 10) have also been developed to represent an "excess function." This function is defined as the isothermal increase in viscosity or thermal conductivity from the low density limit to the real gas density. These correlations are based on the hypothesis that the excess function should only be a function of density. However, recent studies (ref. 6) have shown that, at least for viscosity, this assumption is not valid for high densities (i. e., densities twice critical). A correlation for excess viscosity for both temperature and density effects has been developed by Diller (ref. 6). The correlation is used to calculate real gas viscosities in this report. It is conjectured that further studies will show a similar temperature dependence for thermal conductivity. However, in the absence of available data, the excess thermal conductivity is at present calculated only as a function of density.

In all cases, the real gas transport properties are calculated as an ideal gas value plus an excess function, as shown in the following equations:

$$\mu = \mu_o(T) + A(\rho) \exp \left[\frac{B(\rho)}{T} \right]$$

$$\mu_o(T) = \frac{a_{Ov} T^{3/2} (T + a_{1v})}{(T + a_{2v})(T + a_{3v})}$$

$$A(\rho) = \exp \left[b_{1v} + \ln(\rho) + b_{2v} \rho^{3/2} + b_{3v} \exp(b_{4v} \rho) \right]$$

$$B(\rho) = b_{5v} + b_{6v} \rho^6 + b_{7v} \rho^{3/2} + b_{8v} \exp(b_{9v} \rho^3)$$

$$K = K_o(T) + K_1(\rho)$$

$$K_o(T) = \mu_o^{a_{Ok} + a_{1k}T + C_{p, id}(T)(a_{2k} + a_{3k}T)} m\left(\frac{1 + a_{4k}}{T}\right)$$

$$K_1(\rho) = b_{Ok} + b_{1k}\rho + b_{2k}\rho^2 + b_{2k}\rho^3 + b_{4k}\rho^4 + b_{5k}\rho^5 + b_{6k}\rho^6 + b_{7k}\rho^7 + b_{8k}\rho^8$$

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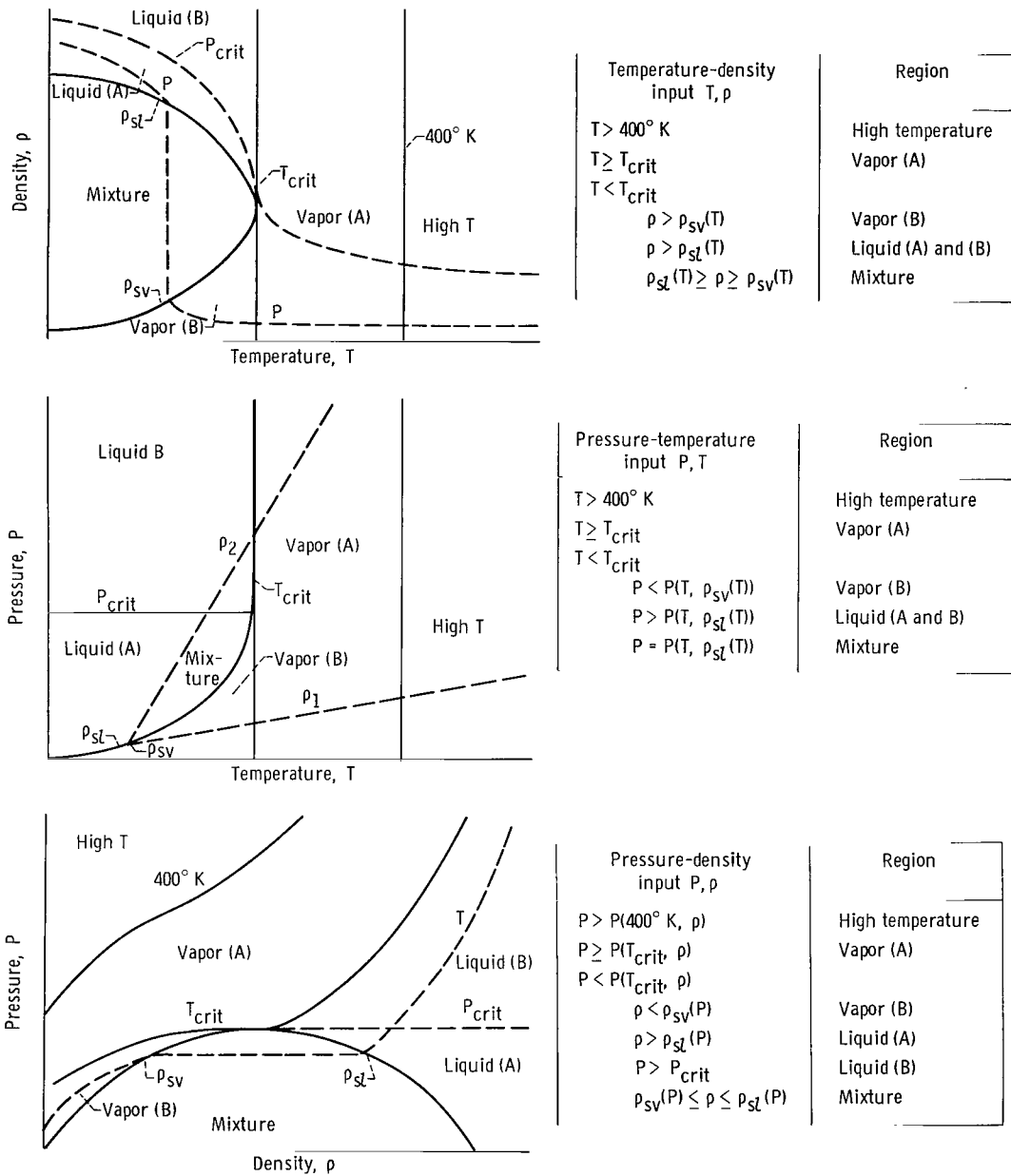


Figure 1. - Region-finding diagrams for pressure-temperature-density input combinations.

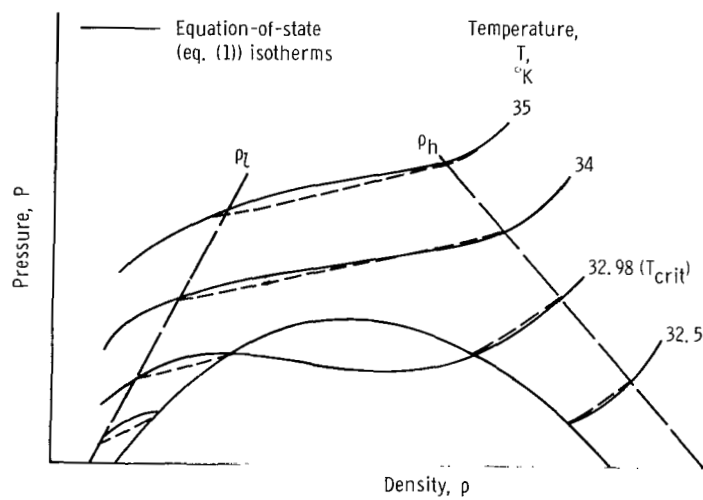


Figure 2. - Critical region represented by approximate isotherms used to give positive derivation (dashed lines).

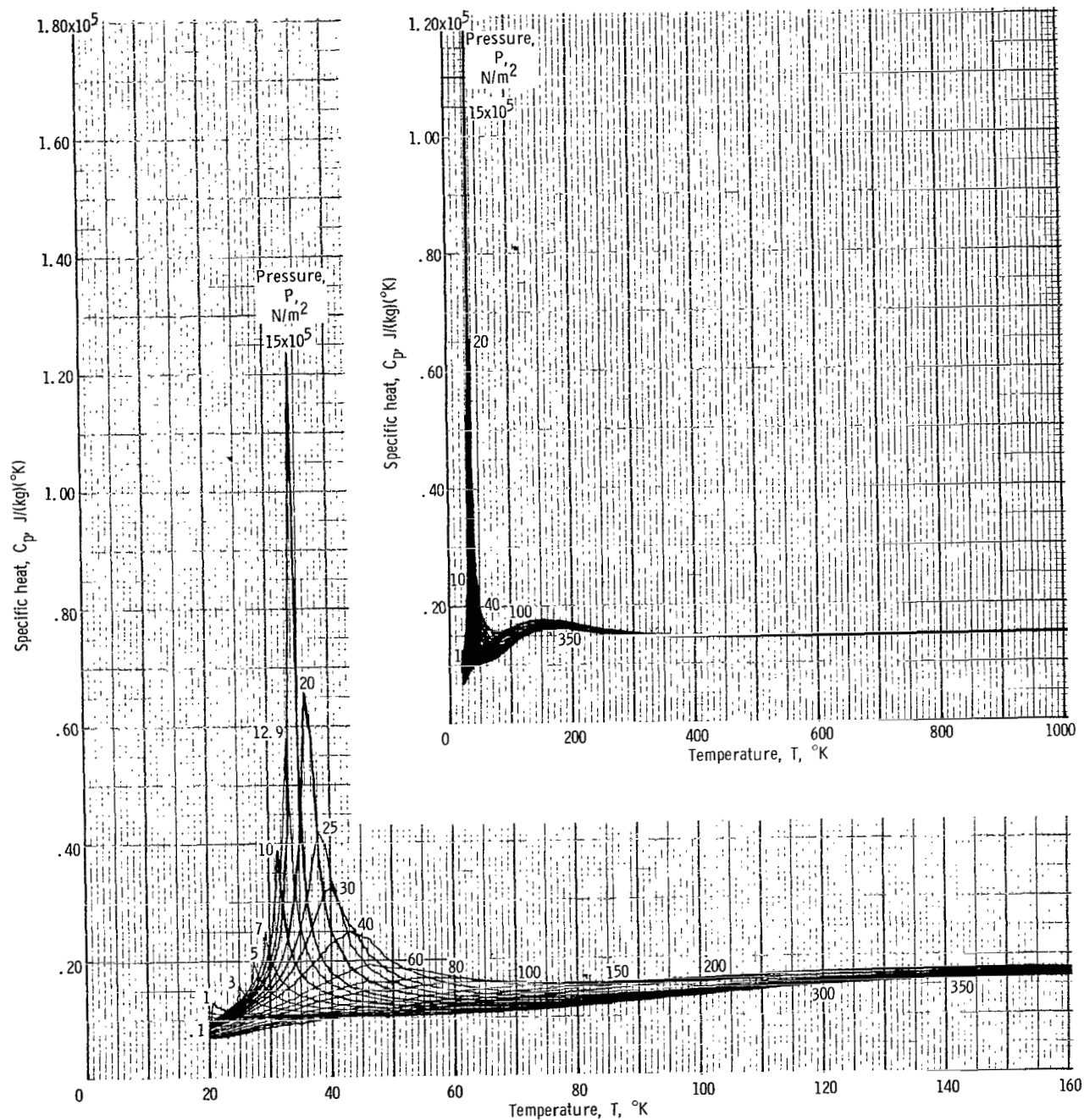


Figure 3. - Specific heat of parahydrogen computer plot from library of functions.

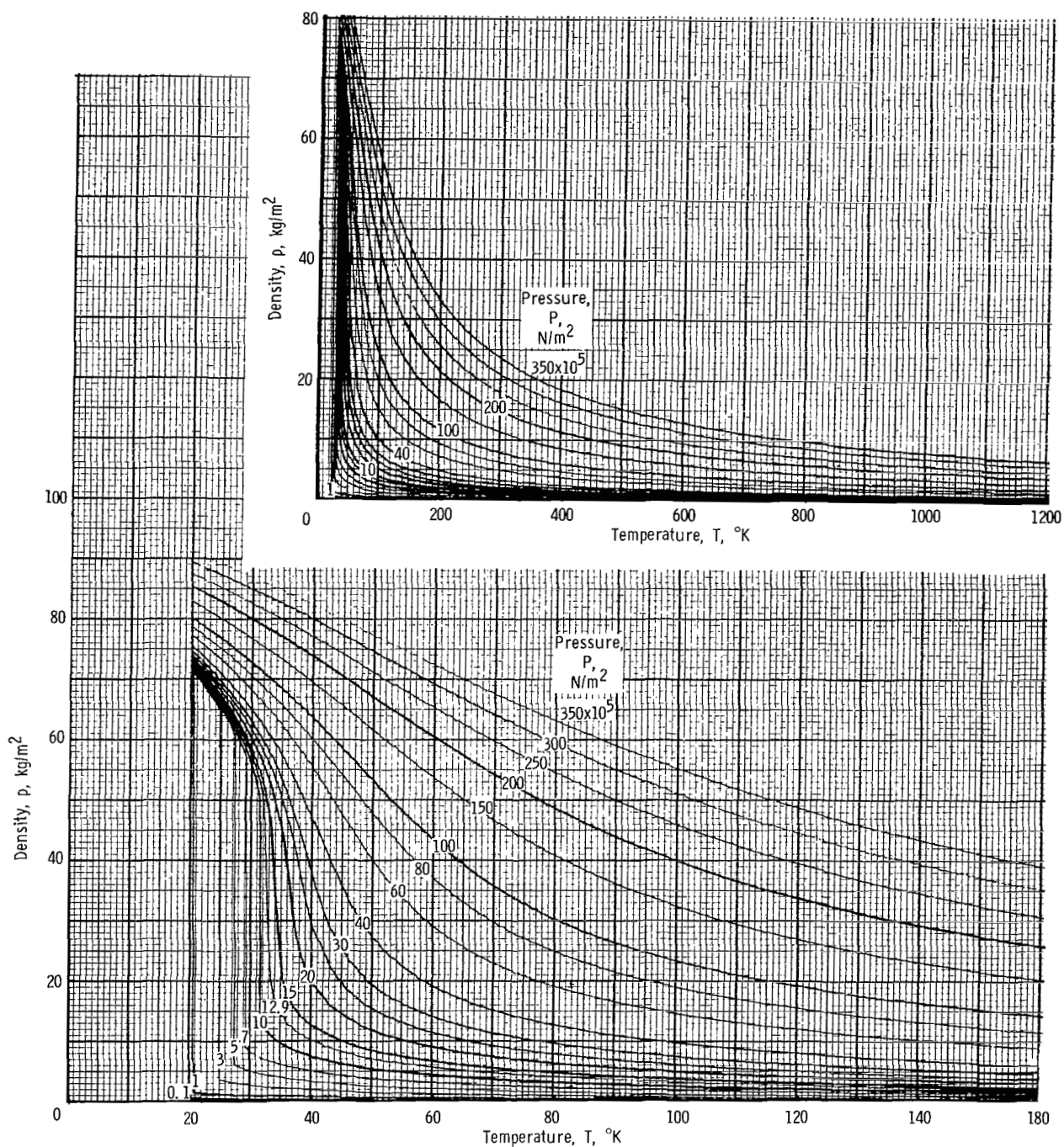


Figure 4. - Density of parahydrogen (computer plot).

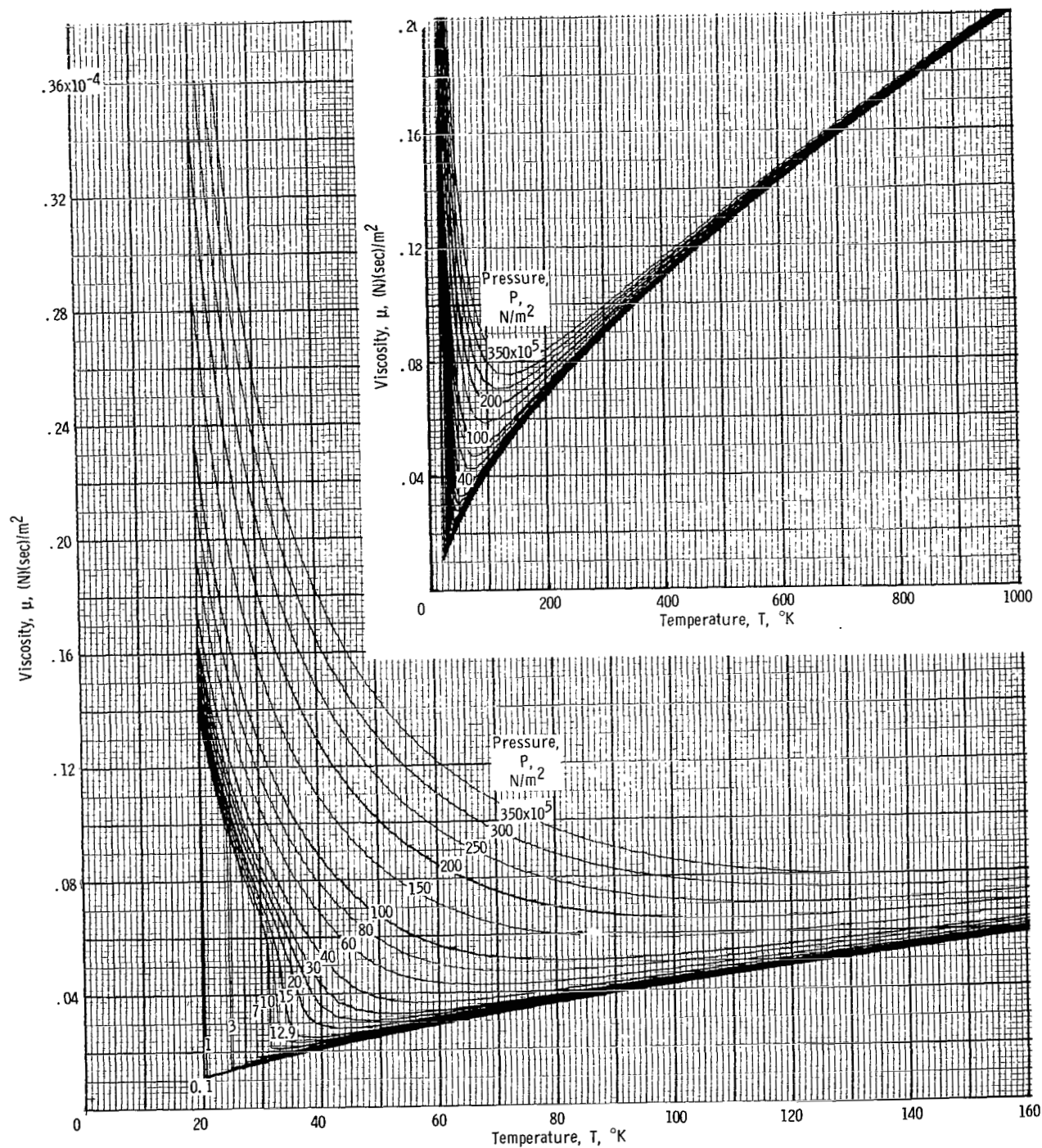


Figure 5. - Viscosity of parahydrogen (computer plot).

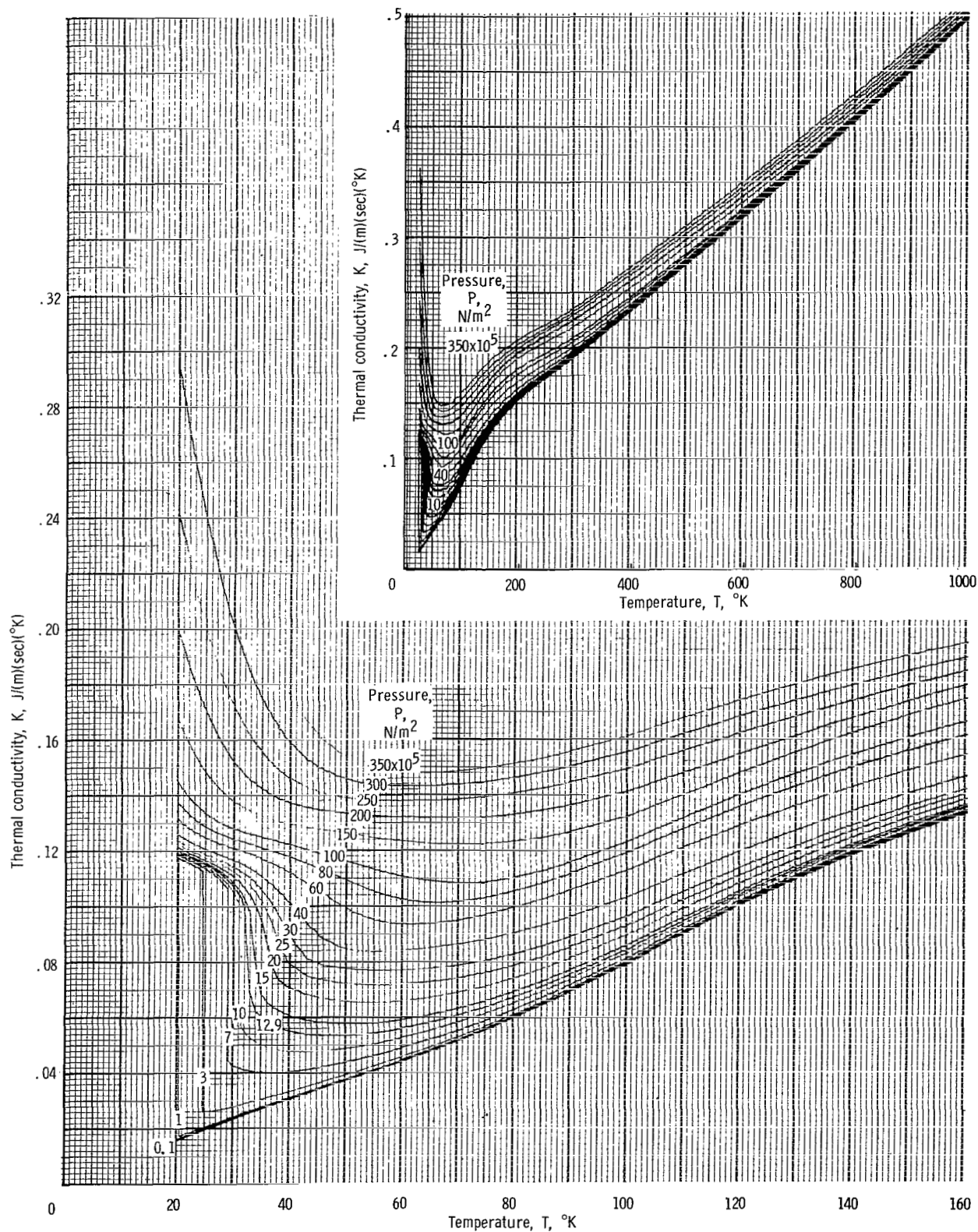


Figure 6. - Thermal conductivity of parahydrogen (computer plot).

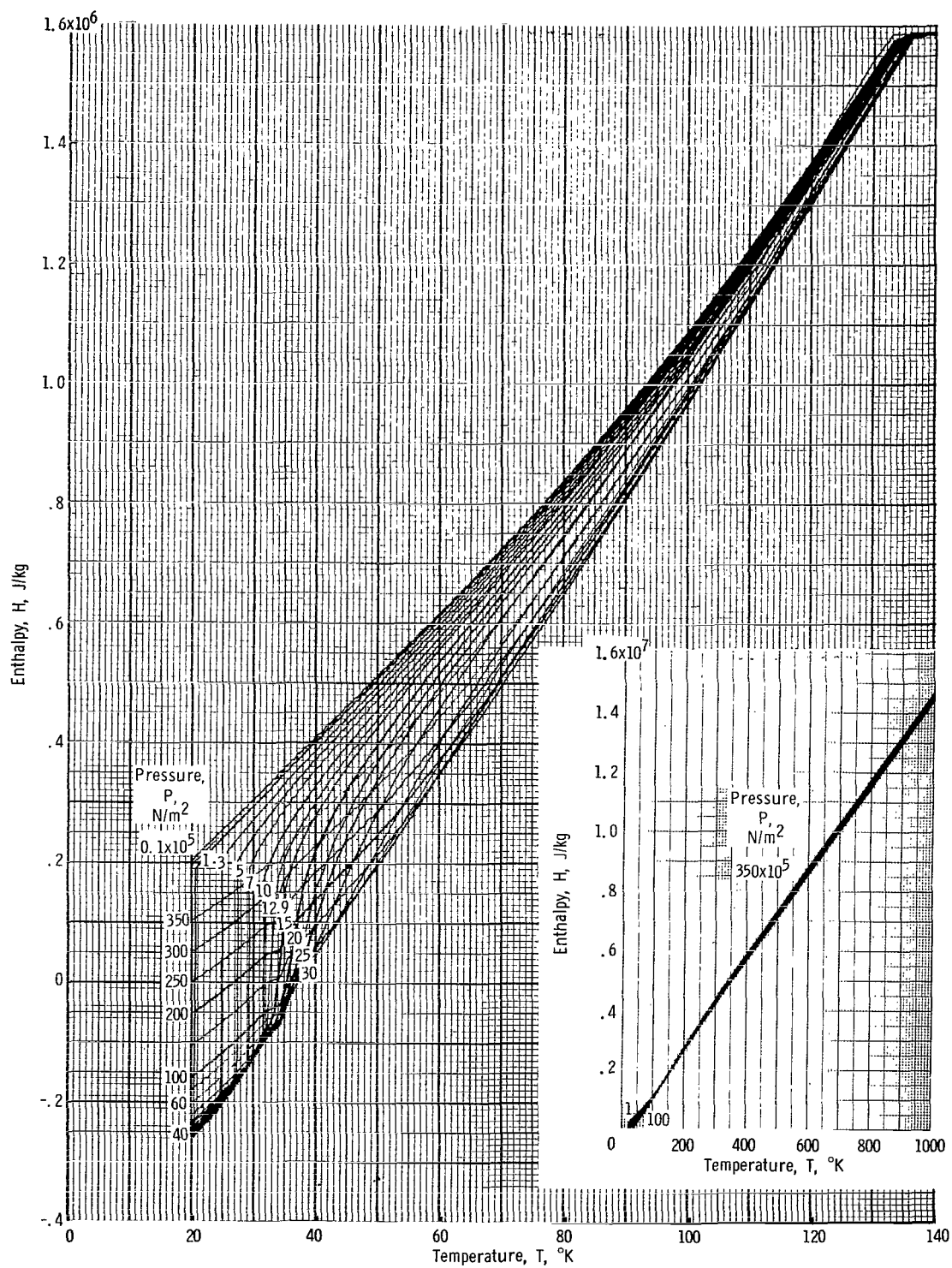


Figure 7. - Enthalpy of parahydrogen (computer plot).

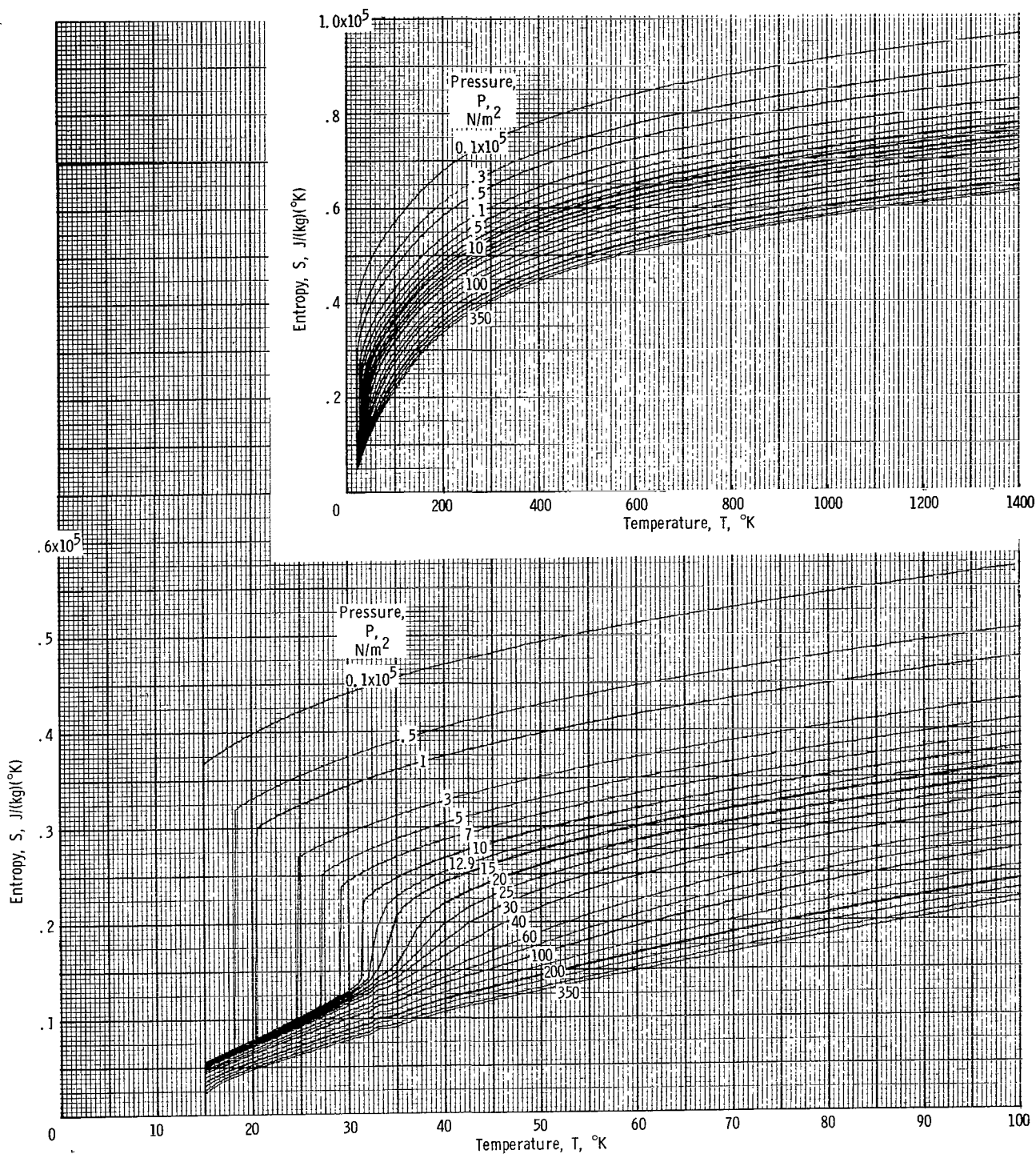


Figure 8. - Entropy of parahydrogen (computer plot).

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